



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:55 PM EDT

PDB ID : 6NLN
Title : 1.60 Å resolution structure of WT BfrB from *Pseudomonas aeruginosa* in complex with a protein-protein interaction inhibitor (analog 16)
Authors : Lovell, S.; Punchi-Hewage, A.; Battaile, K.P.; Yao, H.; Nammalwar, B.; Gnanasekaran, K.K.; Bunce, R.A.; Reitz, A.B.; Rivera, M.
Deposited on : 2019-01-08
Resolution : 1.60 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
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

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 1.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17890 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 Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1272	807	218	240	7	0	1	0
1	B	156	1272	805	217	243	7	0	1	0
1	C	156	1275	807	218	243	7	0	1	0
1	D	156	1281	810	219	245	7	0	1	0
1	E	156	1278	810	218	243	7	0	2	0
1	F	156	1264	802	216	239	7	0	1	0
1	G	156	1269	804	216	242	7	0	1	0
1	H	156	1267	804	217	239	7	0	2	0
1	I	156	1267	803	216	241	7	0	1	0
1	J	156	1268	803	217	241	7	0	1	0
1	K	156	1269	804	216	242	7	0	1	0
1	L	156	1266	803	216	240	7	0	1	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

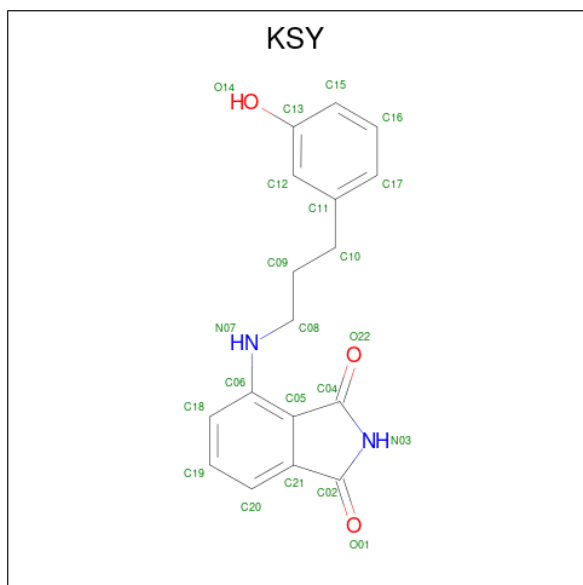
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

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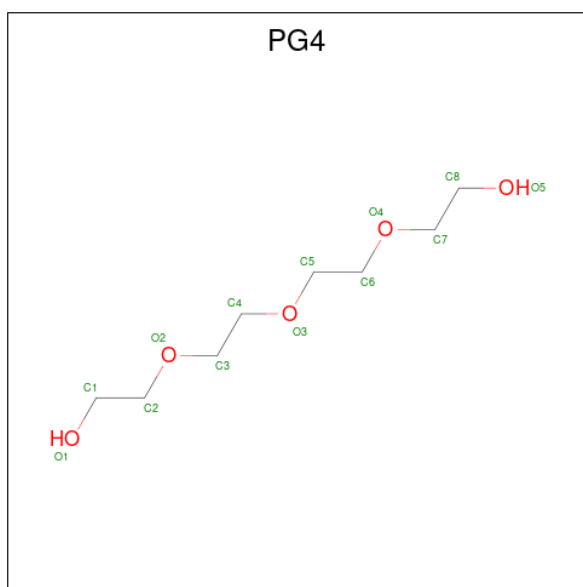
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is 4-{{[3-(3-hydroxyphenyl)propyl]amino}-1H-isoindole-1,3(2H)-dione (three-letter code: KSY) (formula: C₁₇H₁₆N₂O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 22 17 2 3	0	0
3	A	1	Total C N O 22 17 2 3	0	0
3	B	1	Total C N O 22 17 2 3	0	0
3	C	1	Total C N O 22 17 2 3	0	0
3	D	1	Total C N O 22 17 2 3	0	0
3	E	1	Total C N O 22 17 2 3	0	0
3	F	1	Total C N O 22 17 2 3	0	0
3	G	1	Total C N O 22 17 2 3	0	0
3	H	1	Total C N O 16 12 2 2	0	0
3	I	1	Total C N O 22 17 2 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 8 5 3	0	0
5	B	1	Total C O 6 4 2	0	0
5	C	1	Total C O 13 8 5	0	0
5	C	1	Total C O 8 5 3	0	0
5	D	1	Total C O 13 8 5	0	0
5	D	1	Total C O 10 6 4	0	0
5	D	1	Total C O 8 5 3	0	0
5	E	1	Total C O 13 8 5	0	0
5	E	1	Total C O 10 6 4	0	0
5	E	1	Total C O 8 5 3	0	0
5	F	1	Total C O 13 8 5	0	0
5	F	1	Total C O 10 6 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 9 6 3	0	0
5	G	1	Total C O 13 8 5	0	0
5	G	1	Total C O 10 6 4	0	0
5	H	1	Total C O 8 5 3	0	0
5	I	1	Total C O 10 6 4	0	0
5	I	1	Total C O 8 5 3	0	0
5	I	1	Total C O 8 5 3	0	0
5	J	1	Total C O 13 8 5	0	0
5	J	1	Total C O 13 8 5	0	0
5	K	1	Total C O 8 5 3	0	0
5	K	1	Total C O 13 8 5	0	0
5	K	1	Total C O 8 5 3	0	0
5	L	1	Total C O 13 8 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	159	Total O 159 159	0	0
6	B	147	Total O 147 147	0	0
6	C	159	Total O 159 159	0	0
6	D	154	Total O 154 154	0	0
6	E	152	Total O 152 152	0	0
6	F	156	Total O 156 156	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	144	Total 144	O 144	0	0
6	H	152	Total 152	O 152	0	0
6	I	129	Total 129	O 129	0	0
6	J	154	Total 154	O 154	0	0
6	K	154	Total 154	O 154	0	0
6	L	136	Total 136	O 136	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.91Å 194.88Å 203.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 1.60	Depositor
% Data completeness (in resolution range)	100.0 (48.72-1.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.60Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.147 , 0.169	Depositor
Wilson B-factor (Å ²)	18.2	Xtrriage
Anisotropy	0.316	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17890	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 3 are monoatomic - leaving 47 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	B	203	1	41,50,50	1.52	6 (14%)	45,82,82	1.59	11 (24%)
4	HEM	H	202	1	41,50,50	1.55	4 (9%)	45,82,82	1.64	11 (24%)
5	PG4	F	205	-	8,8,12	0.45	0	7,7,11	0.46	0
3	KSY	E	201	-	24,24,24	1.64	5 (20%)	33,33,33	1.21	3 (9%)
3	KSY	B	202	-	24,24,24	1.54	5 (20%)	33,33,33	1.30	3 (9%)
3	KSY	A	203	-	24,24,24	1.77	5 (20%)	33,33,33	1.25	4 (12%)
3	KSY	F	201	-	24,24,24	1.57	5 (20%)	33,33,33	1.33	3 (9%)
5	PG4	E	204	-	7,7,12	0.49	0	6,6,11	0.34	0
3	KSY	A	202	-	24,24,24	1.92	6 (25%)	33,33,33	2.05	6 (18%)
5	PG4	B	204	-	7,7,12	0.57	0	6,6,11	0.22	0
5	PG4	I	202	-	9,9,12	0.37	0	8,8,11	0.59	0
5	PG4	F	204	-	9,9,12	0.55	0	8,8,11	0.31	0
5	PG4	D	206	-	7,7,12	0.41	0	6,6,11	0.32	0
5	PG4	A	205	-	12,12,12	0.46	0	11,11,11	0.42	0
5	PG4	J	203	-	12,12,12	0.43	0	11,11,11	0.49	0
3	KSY	I	201	-	24,24,24	1.62	5 (20%)	33,33,33	1.37	3 (9%)
5	PG4	K	203	-	12,12,12	0.49	0	11,11,11	0.31	0
5	PG4	E	203	-	9,9,12	0.54	0	8,8,11	0.29	0
4	HEM	L	202	1	41,50,50	1.42	3 (7%)	45,82,82	1.39	7 (15%)
4	HEM	C	202	1	41,50,50	1.42	4 (9%)	45,82,82	1.68	13 (28%)
5	PG4	H	203	-	7,7,12	0.51	0	6,6,11	0.28	0
3	KSY	H	201	-	17,17,24	1.94	5 (29%)	23,23,33	1.91	7 (30%)
5	PG4	C	204	-	7,7,12	0.51	0	6,6,11	0.25	0
5	PG4	D	205	-	9,9,12	0.53	0	8,8,11	0.25	0
5	PG4	K	202	-	7,7,12	0.49	0	6,6,11	0.22	0
5	PG4	B	205	-	5,5,12	0.51	0	4,4,11	0.14	0
5	PG4	G	202	-	12,12,12	0.52	0	11,11,11	0.41	0
5	PG4	K	204	-	7,7,12	0.50	0	6,6,11	0.39	0
3	KSY	J	201	-	24,24,24	1.71	5 (20%)	33,33,33	1.72	4 (12%)
3	KSY	K	201	-	16,16,24	2.01	5 (31%)	22,22,33	1.28	2 (9%)
3	KSY	D	202	-	24,24,24	1.80	5 (20%)	33,33,33	1.71	6 (18%)
5	PG4	L	203	-	12,12,12	0.40	0	11,11,11	0.57	0
5	PG4	E	202	-	12,12,12	0.51	0	11,11,11	0.43	0
5	PG4	J	202	-	12,12,12	0.51	0	11,11,11	0.44	0
5	PG4	C	203	-	12,12,12	0.51	0	11,11,11	0.59	0
4	HEM	F	202	1	41,50,50	1.43	4 (9%)	45,82,82	1.47	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	D	204	-	12,12,12	0.49	0	11,11,11	0.45	0
5	PG4	I	204	-	7,7,12	0.38	0	6,6,11	0.45	0
4	HEM	D	203	1	41,50,50	1.46	4 (9%)	45,82,82	1.47	5 (11%)
5	PG4	G	203	-	9,9,12	0.51	0	8,8,11	0.16	0
5	PG4	F	203	-	12,12,12	0.49	0	11,11,11	0.53	0
5	PG4	I	203	-	7,7,12	0.56	0	6,6,11	0.29	0
3	KSY	L	201	-	15,15,24	2.28	6 (40%)	21,21,33	1.90	4 (19%)
5	PG4	A	206	-	9,9,12	0.44	0	8,8,11	0.59	0
4	HEM	A	204	1	41,50,50	1.45	4 (9%)	45,82,82	1.55	11 (24%)
3	KSY	C	201	-	24,24,24	1.65	5 (20%)	33,33,33	1.28	4 (12%)
3	KSY	G	201	-	24,24,24	1.64	5 (20%)	33,33,33	1.12	3 (9%)

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	B	203	1	-	4/12/54/54	-
4	HEM	H	202	1	-	4/12/54/54	-
5	PG4	F	205	-	-	2/6/6/10	-
3	KSY	E	201	-	-	2/7/19/19	0/3/3/3
3	KSY	B	202	-	-	2/7/19/19	0/3/3/3
3	KSY	A	203	-	-	0/7/19/19	0/3/3/3
3	KSY	F	201	-	-	0/7/19/19	0/3/3/3
5	PG4	E	204	-	-	0/5/5/10	-
3	KSY	A	202	-	-	4/7/19/19	0/3/3/3
5	PG4	B	204	-	-	1/5/5/10	-
5	PG4	I	202	-	-	4/7/7/10	-
5	PG4	F	204	-	-	0/7/7/10	-
5	PG4	D	206	-	-	0/5/5/10	-
5	PG4	A	205	-	-	1/10/10/10	-
5	PG4	J	203	-	-	0/10/10/10	-
3	KSY	I	201	-	-	0/7/19/19	0/3/3/3
5	PG4	K	203	-	-	4/10/10/10	-
5	PG4	E	203	-	-	0/7/7/10	-
4	HEM	L	202	1	-	4/12/54/54	-
4	HEM	C	202	1	-	4/12/54/54	-
5	PG4	H	203	-	-	0/5/5/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KSY	H	201	-	-	4/5/17/19	0/2/2/3
5	PG4	C	204	-	-	0/5/5/10	-
5	PG4	D	205	-	-	0/7/7/10	-
5	PG4	K	202	-	-	2/5/5/10	-
5	PG4	B	205	-	-	0/3/3/10	-
5	PG4	G	202	-	-	3/10/10/10	-
5	PG4	K	204	-	-	2/5/5/10	-
3	KSY	J	201	-	-	0/7/19/19	0/3/3/3
3	KSY	K	201	-	-	0/4/16/19	0/2/2/3
3	KSY	D	202	-	-	3/7/19/19	0/3/3/3
5	PG4	L	203	-	-	3/10/10/10	-
5	PG4	E	202	-	-	1/10/10/10	-
5	PG4	J	202	-	-	2/10/10/10	-
5	PG4	C	203	-	-	7/10/10/10	-
4	HEM	F	202	1	-	4/12/54/54	-
5	PG4	D	204	-	-	2/10/10/10	-
5	PG4	I	204	-	-	0/5/5/10	-
4	HEM	D	203	1	-	4/12/54/54	-
5	PG4	G	203	-	-	1/7/7/10	-
5	PG4	F	203	-	-	5/10/10/10	-
5	PG4	I	203	-	-	0/5/5/10	-
3	KSY	L	201	-	-	0/3/15/19	0/2/2/3
5	PG4	A	206	-	-	4/7/7/10	-
4	HEM	A	204	1	-	4/12/54/54	-
3	KSY	C	201	-	-	2/7/19/19	0/3/3/3
3	KSY	G	201	-	-	0/7/19/19	0/3/3/3

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	202	HEM	C3C-C2C	-5.39	1.32	1.40
3	A	202	KSY	C04-N03	5.26	1.46	1.38
4	F	202	HEM	C3C-C2C	-4.88	1.33	1.40
4	B	203	HEM	C3C-C2C	-4.71	1.33	1.40
3	D	202	KSY	C04-N03	4.63	1.45	1.38
3	A	203	KSY	C02-N03	4.58	1.45	1.38
3	A	202	KSY	C21-C02	4.41	1.55	1.48
4	A	204	HEM	C3C-C2C	-4.41	1.34	1.40
3	C	201	KSY	C21-C02	4.38	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	201	KSY	C21-C02	4.34	1.55	1.48
4	D	203	HEM	C3C-C2C	-4.31	1.34	1.40
3	L	201	KSY	C02-N03	4.23	1.44	1.38
3	A	203	KSY	C04-N03	4.23	1.44	1.38
3	L	201	KSY	C04-N03	4.18	1.44	1.38
3	D	202	KSY	C02-N03	4.17	1.44	1.38
3	I	201	KSY	C21-C02	4.14	1.54	1.48
3	K	201	KSY	C21-C02	4.02	1.54	1.48
3	J	201	KSY	C02-N03	3.87	1.44	1.38
3	H	201	KSY	C21-C02	3.86	1.54	1.48
3	D	202	KSY	C21-C02	3.83	1.54	1.48
3	G	201	KSY	C21-C02	3.83	1.54	1.48
3	E	201	KSY	C04-N03	3.79	1.44	1.38
4	C	202	HEM	C3C-C2C	-3.79	1.35	1.40
3	A	202	KSY	C02-N03	3.79	1.44	1.38
4	L	202	HEM	C3C-C2C	-3.78	1.35	1.40
3	J	201	KSY	C04-N03	3.76	1.44	1.38
3	H	201	KSY	C04-N03	3.69	1.44	1.38
4	L	202	HEM	C3C-CAC	3.66	1.55	1.47
3	E	201	KSY	C21-C02	3.65	1.54	1.48
3	K	201	KSY	C04-N03	3.61	1.43	1.38
3	E	201	KSY	C02-N03	3.56	1.43	1.38
4	H	202	HEM	C3C-CAC	3.52	1.55	1.47
3	G	201	KSY	C06-N07	3.49	1.47	1.37
3	H	201	KSY	C06-N07	3.49	1.47	1.37
4	D	203	HEM	C3C-CAC	3.46	1.54	1.47
3	A	203	KSY	C21-C02	3.43	1.53	1.48
3	F	201	KSY	C04-N03	3.40	1.43	1.38
3	J	201	KSY	C06-N07	3.38	1.46	1.37
3	K	201	KSY	C06-N07	3.35	1.46	1.37
3	F	201	KSY	C02-N03	3.32	1.43	1.38
4	C	202	HEM	C3C-CAC	3.30	1.54	1.47
3	I	201	KSY	C04-N03	3.30	1.43	1.38
3	B	202	KSY	C21-C02	3.28	1.53	1.48
3	I	201	KSY	C02-N03	3.23	1.43	1.38
3	J	201	KSY	C21-C02	3.23	1.53	1.48
3	B	202	KSY	C06-N07	3.20	1.46	1.37
3	C	201	KSY	C06-N07	3.19	1.46	1.37
3	C	201	KSY	C04-N03	3.18	1.43	1.38
3	F	201	KSY	C06-N07	3.17	1.46	1.37
4	F	202	HEM	C3C-CAC	3.14	1.54	1.47
3	K	201	KSY	C02-N03	3.11	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	201	KSY	C04-N03	3.11	1.43	1.38
3	F	201	KSY	C21-C02	3.11	1.53	1.48
3	B	202	KSY	C04-N03	3.03	1.43	1.38
3	I	201	KSY	C06-N07	2.98	1.45	1.37
4	B	203	HEM	C3C-CAC	2.96	1.53	1.47
3	A	203	KSY	C06-N07	2.95	1.45	1.37
3	H	201	KSY	C02-N03	2.93	1.43	1.38
3	D	202	KSY	C06-N07	2.91	1.45	1.37
3	L	201	KSY	C06-N07	2.83	1.45	1.37
4	A	204	HEM	C3C-CAC	2.83	1.53	1.47
3	A	202	KSY	C06-N07	2.81	1.45	1.37
3	B	202	KSY	C02-N03	2.80	1.42	1.38
3	G	201	KSY	O01-C02	-2.79	1.17	1.23
3	E	201	KSY	C06-N07	2.74	1.45	1.37
4	L	202	HEM	CAB-C3B	2.70	1.54	1.47
4	A	204	HEM	CAB-C3B	2.69	1.54	1.47
4	C	202	HEM	CAB-C3B	2.65	1.54	1.47
3	C	201	KSY	C02-N03	2.62	1.42	1.38
4	D	203	HEM	CAB-C3B	2.57	1.54	1.47
3	C	201	KSY	O01-C02	-2.53	1.18	1.23
4	H	202	HEM	CAB-C3B	2.51	1.54	1.47
3	G	201	KSY	C02-N03	2.50	1.42	1.38
3	J	201	KSY	O01-C02	-2.49	1.18	1.23
3	B	202	KSY	O01-C02	-2.45	1.18	1.23
3	I	201	KSY	O01-C02	-2.44	1.18	1.23
3	E	201	KSY	O01-C02	-2.42	1.18	1.23
3	K	201	KSY	O01-C02	-2.42	1.18	1.23
4	H	202	HEM	CAA-C2A	2.41	1.55	1.52
3	A	202	KSY	O01-C02	-2.41	1.18	1.23
3	D	202	KSY	O01-C02	-2.40	1.18	1.23
4	F	202	HEM	CAB-C3B	2.40	1.54	1.47
3	H	201	KSY	O01-C02	-2.40	1.18	1.23
4	B	203	HEM	CMB-C2B	2.39	1.55	1.50
3	L	201	KSY	O01-C02	-2.38	1.18	1.23
4	B	203	HEM	CAB-C3B	2.36	1.53	1.47
4	C	202	HEM	CMD-C2D	2.27	1.55	1.50
4	D	203	HEM	CMD-C2D	2.21	1.55	1.50
3	A	203	KSY	O22-C04	-2.20	1.18	1.23
3	L	201	KSY	O22-C04	-2.19	1.18	1.23
4	F	202	HEM	CMD-C2D	2.14	1.55	1.50
4	A	204	HEM	CMD-C2D	2.11	1.55	1.50
3	F	201	KSY	O01-C02	-2.10	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	203	HEM	CAA-C2A	2.08	1.55	1.52
4	B	203	HEM	CMD-C2D	2.08	1.55	1.50
3	A	202	KSY	O22-C04	-2.01	1.19	1.23

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	KSY	C04-N03-C02	-8.24	105.49	112.52
3	D	202	KSY	C04-N03-C02	-7.02	106.53	112.52
3	L	201	KSY	C04-N03-C02	-5.97	107.43	112.52
3	J	201	KSY	C05-C06-N07	-5.52	114.77	121.32
3	H	201	KSY	C21-C05-C06	-5.52	118.11	121.91
3	J	201	KSY	C04-N03-C02	-5.48	107.85	112.52
3	A	202	KSY	C21-C02-N03	4.68	110.19	105.89
3	A	203	KSY	C04-N03-C02	-4.56	108.64	112.52
4	D	203	HEM	CBA-CAA-C2A	-4.03	105.74	112.62
3	I	201	KSY	C21-C05-C06	-3.99	119.16	121.91
3	I	201	KSY	C05-C06-N07	-3.99	116.60	121.32
3	A	202	KSY	C05-C06-N07	-3.95	116.64	121.32
3	C	201	KSY	C05-C06-N07	-3.83	116.78	121.32
3	B	202	KSY	C21-C05-C06	-3.79	119.30	121.91
3	F	201	KSY	C05-C06-N07	-3.70	116.94	121.32
3	H	201	KSY	C06-C05-C04	3.66	134.37	129.21
3	B	202	KSY	C05-C06-N07	-3.66	116.99	121.32
4	C	202	HEM	C4D-ND-C1D	3.64	108.83	105.07
3	L	201	KSY	C05-C06-N07	-3.61	117.04	121.32
3	D	202	KSY	C21-C02-N03	3.51	109.12	105.89
3	G	201	KSY	C05-C06-N07	-3.48	117.20	121.32
4	H	202	HEM	C4D-ND-C1D	3.46	108.64	105.07
4	B	203	HEM	C1B-NB-C4B	3.43	108.61	105.07
3	J	201	KSY	C21-C02-N03	3.40	109.01	105.89
3	A	202	KSY	C21-C05-C06	-3.22	119.69	121.91
4	H	202	HEM	CMA-C3A-C4A	-3.22	123.52	128.46
3	K	201	KSY	C05-C06-N07	-3.21	117.51	121.32
4	H	202	HEM	C1B-NB-C4B	3.19	108.37	105.07
3	F	201	KSY	C21-C05-C06	-3.18	119.72	121.91
4	B	203	HEM	CBA-CAA-C2A	-3.17	107.21	112.62
3	C	201	KSY	C21-C05-C06	-3.15	119.74	121.91
4	B	203	HEM	C4D-ND-C1D	3.12	108.30	105.07
4	D	203	HEM	C4D-ND-C1D	3.09	108.27	105.07
4	B	203	HEM	C4B-CHC-C1C	3.08	126.63	122.56
3	E	201	KSY	C21-C05-C06	-3.08	119.79	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	201	KSY	C21-C02-N03	3.05	108.69	105.89
4	F	202	HEM	CMA-C3A-C4A	-3.04	123.79	128.46
3	H	201	KSY	C05-C06-N07	3.04	124.92	121.32
4	C	202	HEM	CMC-C2C-C3C	3.03	130.34	124.68
4	H	202	HEM	C4B-C3B-C2B	2.99	109.49	107.11
3	E	201	KSY	C05-C06-N07	-2.99	117.78	121.32
4	A	204	HEM	C4B-CHC-C1C	2.98	126.49	122.56
4	L	202	HEM	C4D-ND-C1D	2.98	108.15	105.07
4	A	204	HEM	CBA-CAA-C2A	-2.91	107.66	112.62
4	D	203	HEM	C4C-CHD-C1D	2.88	126.35	122.56
3	B	202	KSY	O22-C04-C05	2.88	132.83	128.55
4	A	204	HEM	C4D-ND-C1D	2.87	108.04	105.07
3	H	201	KSY	C18-C06-N07	-2.86	116.92	121.80
4	A	204	HEM	C4C-CHD-C1D	2.84	126.30	122.56
4	A	204	HEM	CMA-C3A-C4A	-2.83	124.12	128.46
3	G	201	KSY	O22-C04-C05	2.82	132.75	128.55
4	H	202	HEM	CHC-C4B-NB	2.80	127.47	124.43
3	E	201	KSY	C04-N03-C02	-2.76	110.17	112.52
3	J	201	KSY	C18-C06-N07	2.73	126.45	121.80
4	H	202	HEM	C4B-CHC-C1C	2.71	126.14	122.56
4	F	202	HEM	C2C-C3C-C4C	2.65	108.75	106.90
4	H	202	HEM	C2C-C3C-C4C	2.65	108.75	106.90
4	B	203	HEM	C2C-C3C-C4C	2.61	108.72	106.90
4	A	204	HEM	CMC-C2C-C3C	2.60	129.55	124.68
4	L	202	HEM	CMC-C2C-C3C	2.58	129.50	124.68
4	C	202	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
4	C	202	HEM	CAD-CBD-CGD	-2.57	108.08	113.60
3	K	201	KSY	C21-C05-C06	-2.55	120.16	121.91
4	F	202	HEM	C4D-ND-C1D	2.51	107.66	105.07
4	C	202	HEM	C2D-C1D-ND	-2.51	106.88	109.88
4	C	202	HEM	C4B-CHC-C1C	2.50	125.85	122.56
4	F	202	HEM	CAD-CBD-CGD	-2.49	108.25	113.60
4	A	204	HEM	C2C-C3C-C4C	2.46	108.62	106.90
4	C	202	HEM	C1B-NB-C4B	2.43	107.58	105.07
4	C	202	HEM	C3D-C4D-ND	-2.43	107.46	110.17
4	L	202	HEM	CMA-C3A-C4A	-2.43	124.73	128.46
3	H	201	KSY	C04-N03-C02	-2.41	110.47	112.52
4	C	202	HEM	CHD-C1D-ND	2.39	127.03	124.43
4	F	202	HEM	C4C-CHD-C1D	2.39	125.72	122.56
3	D	202	KSY	C21-C05-C06	-2.39	120.26	121.91
3	A	202	KSY	C06-C05-C04	2.38	132.56	129.21
3	D	202	KSY	C05-C06-N07	-2.36	118.52	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	202	HEM	CBA-CAA-C2A	-2.34	108.63	112.62
4	L	202	HEM	CBA-CAA-C2A	-2.32	108.66	112.62
4	C	202	HEM	C2C-C3C-C4C	2.31	108.51	106.90
4	H	202	HEM	C4A-C3A-C2A	2.29	108.59	107.00
4	C	202	HEM	C4A-C3A-C2A	2.28	108.58	107.00
3	D	202	KSY	O22-C04-C05	-2.26	125.18	128.55
3	L	201	KSY	C21-C05-C06	-2.26	120.36	121.91
4	D	203	HEM	CMC-C2C-C3C	2.25	128.89	124.68
4	L	202	HEM	C4C-CHD-C1D	2.25	125.53	122.56
3	I	201	KSY	O22-C04-C05	2.24	131.88	128.55
3	A	202	KSY	O22-C04-C05	-2.21	125.26	128.55
4	L	202	HEM	C3D-C4D-ND	-2.20	107.71	110.17
3	H	201	KSY	O22-C04-C05	2.20	131.82	128.55
4	D	203	HEM	C4B-CHC-C1C	2.20	125.46	122.56
4	A	204	HEM	C4A-C3A-C2A	2.19	108.52	107.00
3	G	201	KSY	C21-C05-C06	-2.19	120.40	121.91
4	A	204	HEM	C3D-C4D-ND	-2.19	107.72	110.17
3	A	203	KSY	C08-N07-C06	-2.19	118.12	123.39
4	F	202	HEM	CBA-CAA-C2A	-2.19	108.89	112.62
3	A	203	KSY	O22-C04-C05	-2.17	125.32	128.55
3	F	201	KSY	O22-C04-C05	2.17	131.78	128.55
4	B	203	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
3	H	201	KSY	C19-C18-C06	2.16	123.10	118.62
4	C	202	HEM	CHC-C4B-NB	2.13	126.75	124.43
4	B	203	HEM	C3D-C4D-ND	-2.13	107.79	110.17
4	A	204	HEM	C4B-C3B-C2B	2.13	108.80	107.11
4	L	202	HEM	C1B-NB-C4B	2.12	107.26	105.07
4	C	202	HEM	CBA-CAA-C2A	-2.10	109.04	112.62
4	B	203	HEM	C4B-C3B-C2B	2.10	108.78	107.11
4	H	202	HEM	C3D-C4D-ND	-2.09	107.84	110.17
4	B	203	HEM	CHB-C1B-NB	2.08	126.96	124.38
4	A	204	HEM	CBD-CAD-C3D	-2.07	106.87	112.63
3	A	203	KSY	C21-C05-C06	-2.06	120.49	121.91
3	D	202	KSY	C06-C05-C04	2.06	132.11	129.21
4	B	203	HEM	CHC-C4B-C3B	2.04	127.69	124.57
4	H	202	HEM	C2D-C1D-ND	-2.03	107.45	109.88
4	B	203	HEM	CAD-CBD-CGD	-2.03	109.25	113.60
3	C	201	KSY	C04-N03-C02	-2.02	110.80	112.52
3	C	201	KSY	O22-C04-C05	2.01	131.53	128.55

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	201	KSY	C18-C06-N07-C08
3	H	201	KSY	C05-C06-N07-C08
5	I	202	PG4	O4-C7-C8-O5
3	H	201	KSY	N07-C08-C09-C10
5	I	202	PG4	O3-C5-C6-O4
5	A	206	PG4	O2-C3-C4-O3
5	K	204	PG4	O2-C3-C4-O3
5	F	203	PG4	O2-C3-C4-O3
5	F	203	PG4	O3-C5-C6-O4
5	C	203	PG4	O3-C5-C6-O4
3	D	202	KSY	N07-C08-C09-C10
5	C	203	PG4	O2-C3-C4-O3
5	C	203	PG4	O4-C7-C8-O5
5	D	204	PG4	O4-C7-C8-O5
5	F	203	PG4	O1-C1-C2-O2
5	A	206	PG4	O1-C1-C2-O2
5	F	205	PG4	O2-C3-C4-O3
5	E	202	PG4	O3-C5-C6-O4
3	H	201	KSY	C08-C09-C10-C11
3	A	202	KSY	N07-C08-C09-C10
5	G	202	PG4	O4-C7-C8-O5
5	L	203	PG4	O4-C7-C8-O5
5	K	202	PG4	O4-C7-C8-O5
5	K	203	PG4	O3-C5-C6-O4
5	K	202	PG4	O3-C5-C6-O4
5	D	204	PG4	O3-C5-C6-O4
5	K	203	PG4	O1-C1-C2-O2
5	L	203	PG4	O1-C1-C2-O2
5	I	202	PG4	C5-C6-O4-C7
5	A	206	PG4	C3-C4-O3-C5
5	A	206	PG4	C6-C5-O3-C4
5	J	202	PG4	O1-C1-C2-O2
5	G	202	PG4	O3-C5-C6-O4
5	G	202	PG4	C8-C7-O4-C6
5	J	202	PG4	O3-C5-C6-O4
5	B	204	PG4	O4-C7-C8-O5
5	C	203	PG4	C8-C7-O4-C6
5	K	203	PG4	C1-C2-O2-C3
5	F	205	PG4	C3-C4-O3-C5
5	A	205	PG4	O3-C5-C6-O4
5	I	202	PG4	C3-C4-O3-C5
5	C	203	PG4	C1-C2-O2-C3
5	F	203	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
5	C	203	PG4	C6-C5-O3-C4
5	C	203	PG4	C5-C6-O4-C7
3	A	202	KSY	C09-C10-C11-C12
3	E	201	KSY	C09-C10-C11-C17
4	B	203	HEM	CAD-CBD-CGD-O1D
4	C	202	HEM	CAD-CBD-CGD-O2D
4	F	202	HEM	CAD-CBD-CGD-O1D
4	B	203	HEM	CAD-CBD-CGD-O2D
3	B	202	KSY	C09-C10-C11-C17
4	L	202	HEM	CAD-CBD-CGD-O2D
3	A	202	KSY	C09-C10-C11-C17
3	E	201	KSY	C09-C10-C11-C12
4	F	202	HEM	CAD-CBD-CGD-O2D
4	A	204	HEM	CAD-CBD-CGD-O1D
3	B	202	KSY	C09-C10-C11-C12
4	H	202	HEM	CAA-CBA-CGA-O2A
4	H	202	HEM	CAD-CBD-CGD-O2D
4	A	204	HEM	CAA-CBA-CGA-O1A
4	H	202	HEM	CAD-CBD-CGD-O1D
3	D	202	KSY	C09-C10-C11-C12
4	A	204	HEM	CAD-CBD-CGD-O2D
4	B	203	HEM	CAA-CBA-CGA-O1A
4	D	203	HEM	CAD-CBD-CGD-O1D
5	K	204	PG4	C4-C3-O2-C2
4	L	202	HEM	CAD-CBD-CGD-O1D
3	C	201	KSY	C09-C10-C11-C17
4	A	204	HEM	CAA-CBA-CGA-O2A
4	C	202	HEM	CAD-CBD-CGD-O1D
4	D	203	HEM	CAD-CBD-CGD-O2D
4	H	202	HEM	CAA-CBA-CGA-O1A
3	C	201	KSY	C09-C10-C11-C12
5	K	203	PG4	O2-C3-C4-O3
3	D	202	KSY	C09-C10-C11-C17
4	B	203	HEM	CAA-CBA-CGA-O2A
4	C	202	HEM	CAA-CBA-CGA-O2A
4	F	202	HEM	CAA-CBA-CGA-O2A
4	C	202	HEM	CAA-CBA-CGA-O1A
4	D	203	HEM	CAA-CBA-CGA-O2A
4	F	202	HEM	CAA-CBA-CGA-O1A
4	L	202	HEM	CAA-CBA-CGA-O2A
4	D	203	HEM	CAA-CBA-CGA-O1A
4	L	202	HEM	CAA-CBA-CGA-O1A

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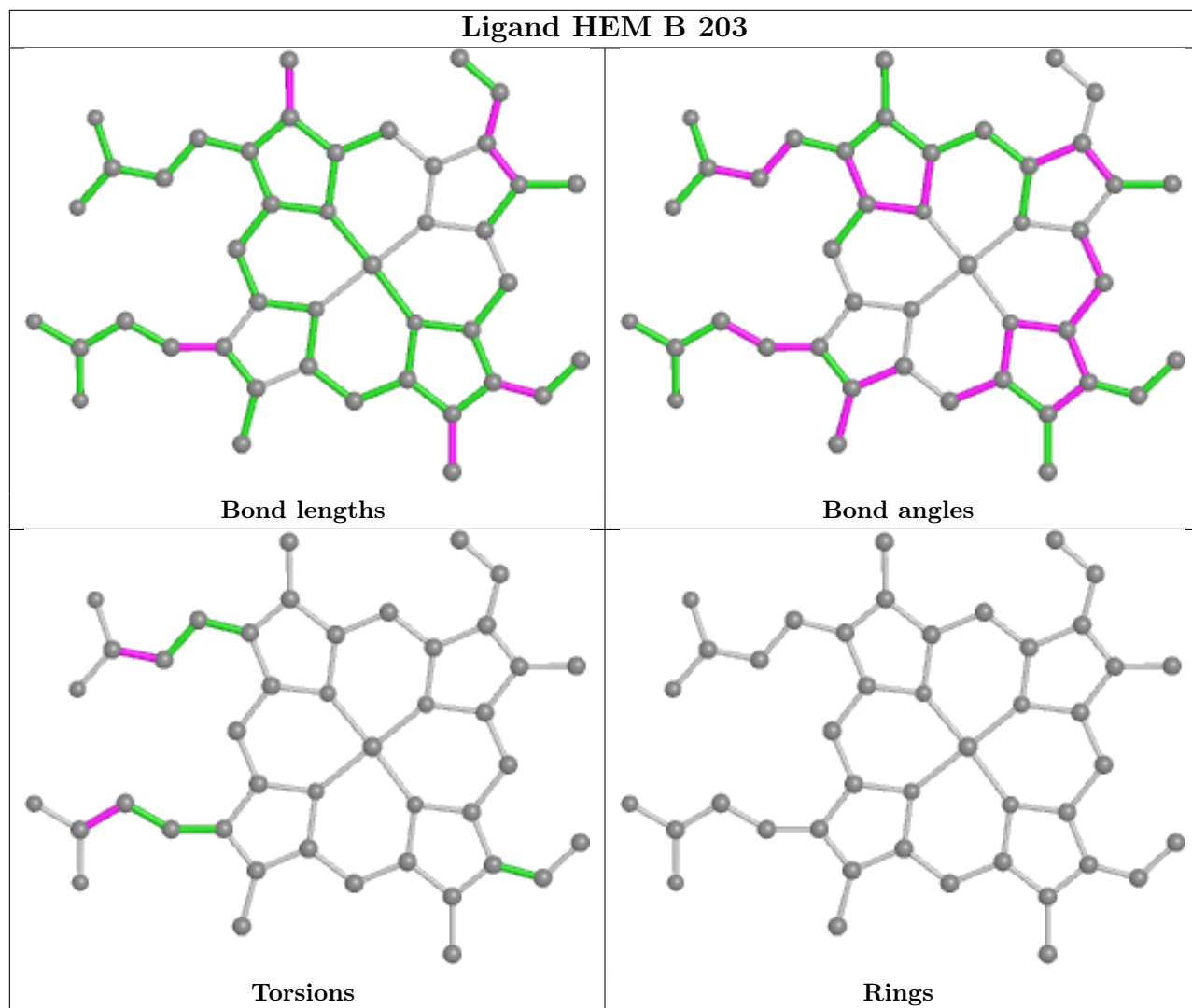
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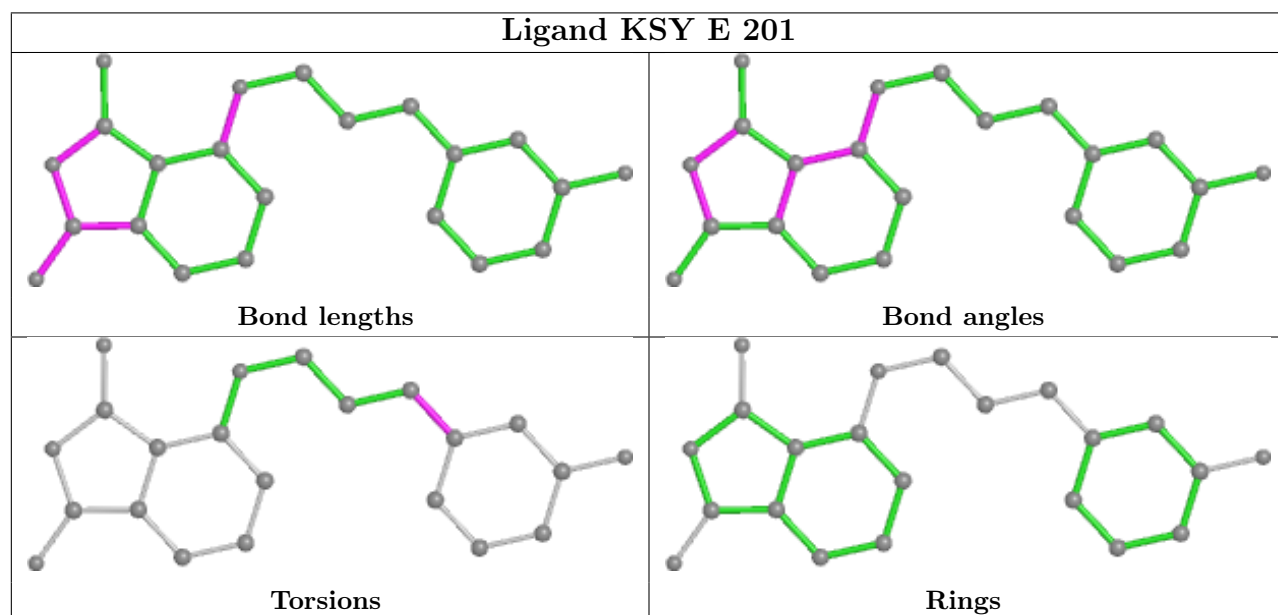
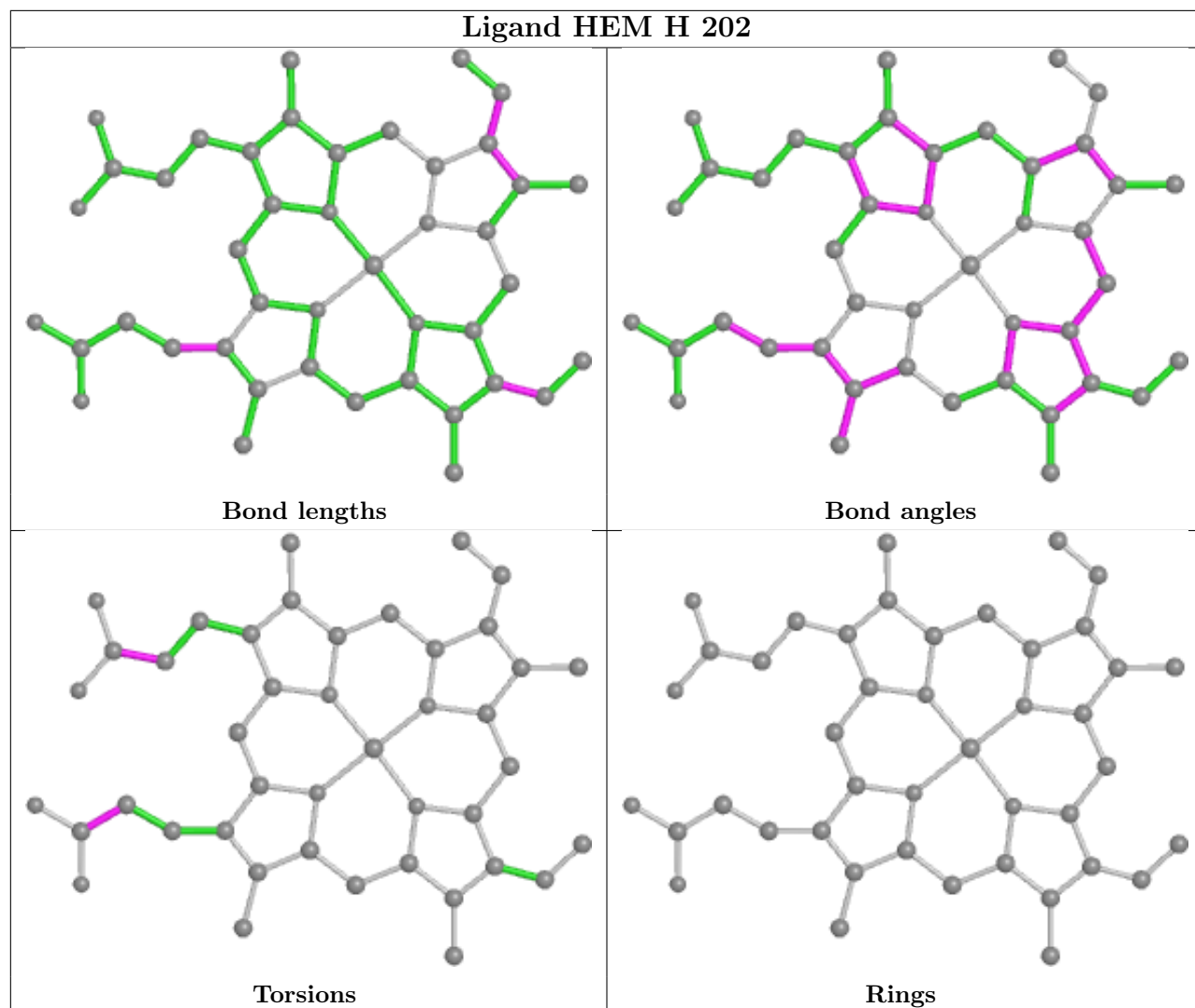
Mol	Chain	Res	Type	Atoms
5	L	203	PG4	O2-C3-C4-O3
3	A	202	KSY	C08-C09-C10-C11
5	G	203	PG4	C8-C7-O4-C6
5	F	203	PG4	O4-C7-C8-O5

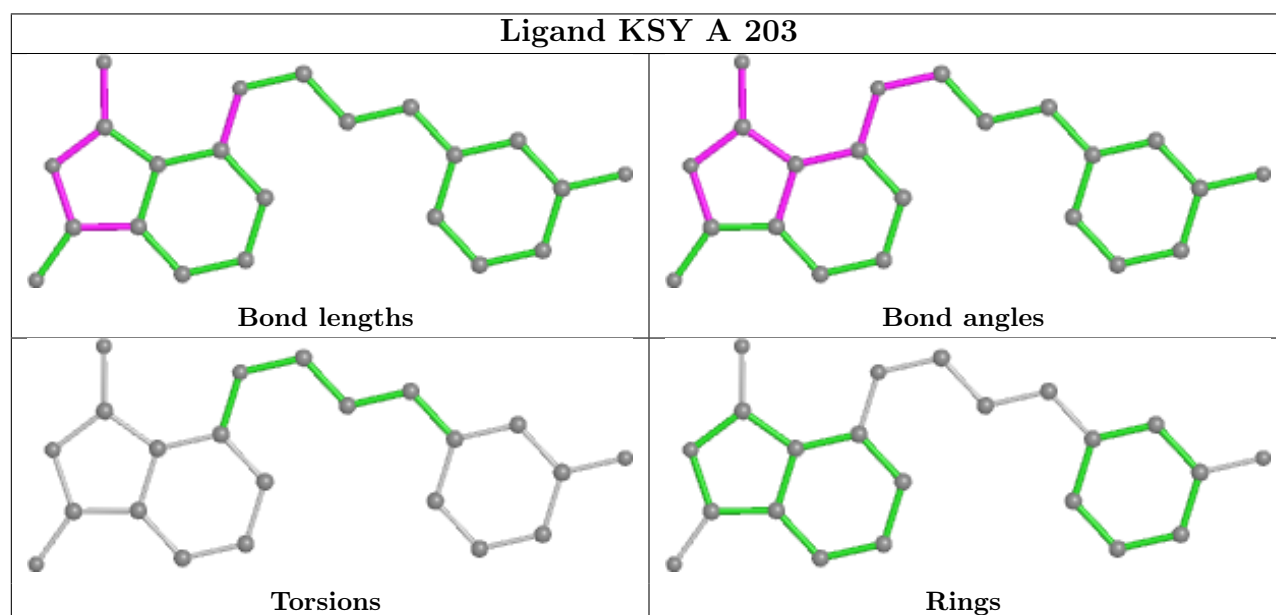
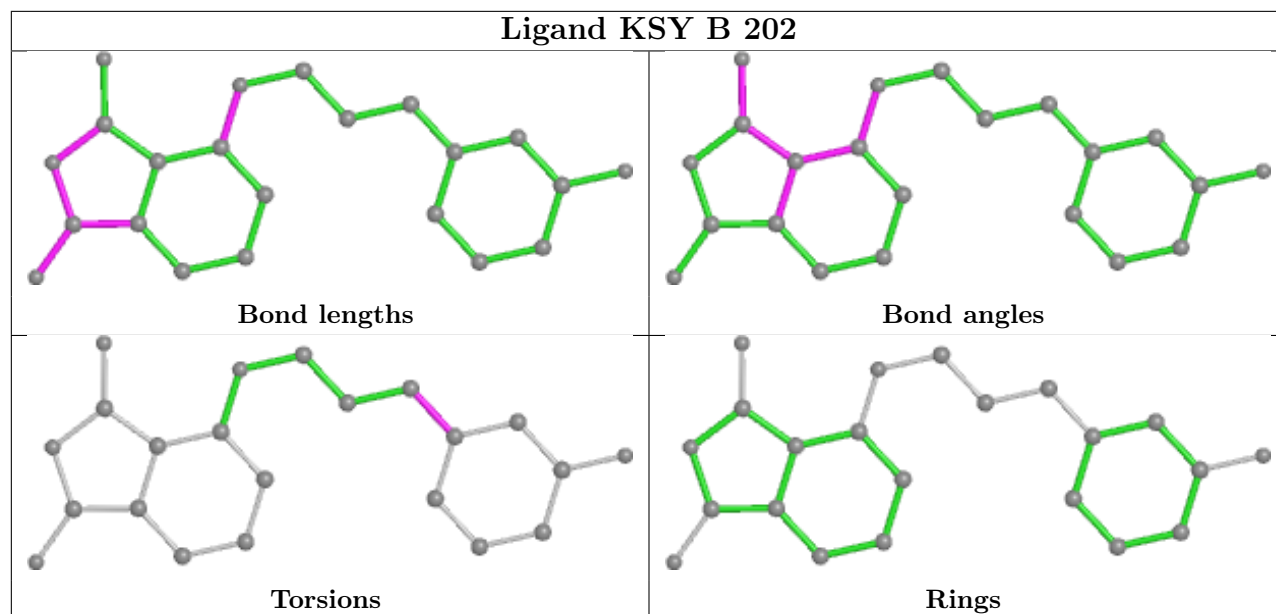
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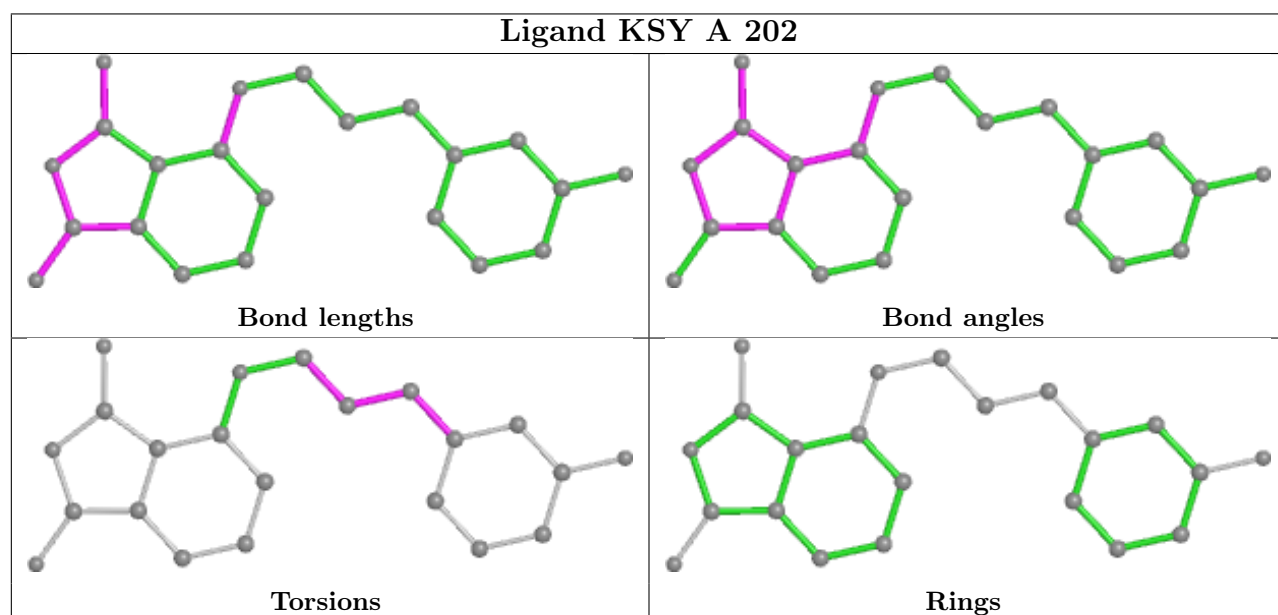
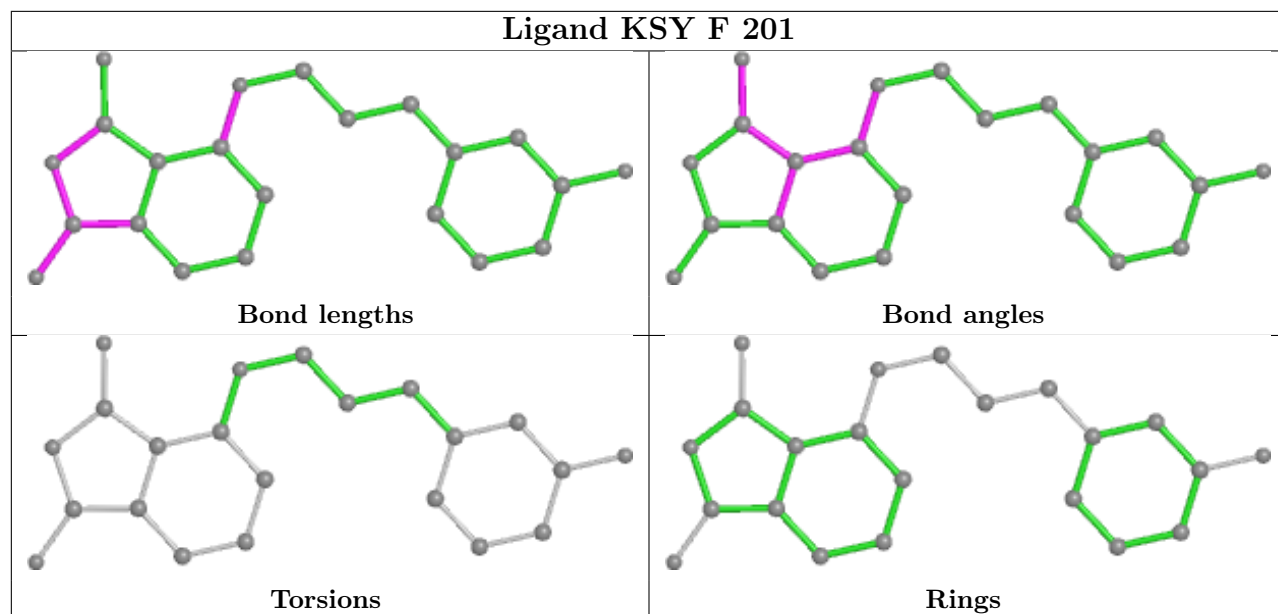
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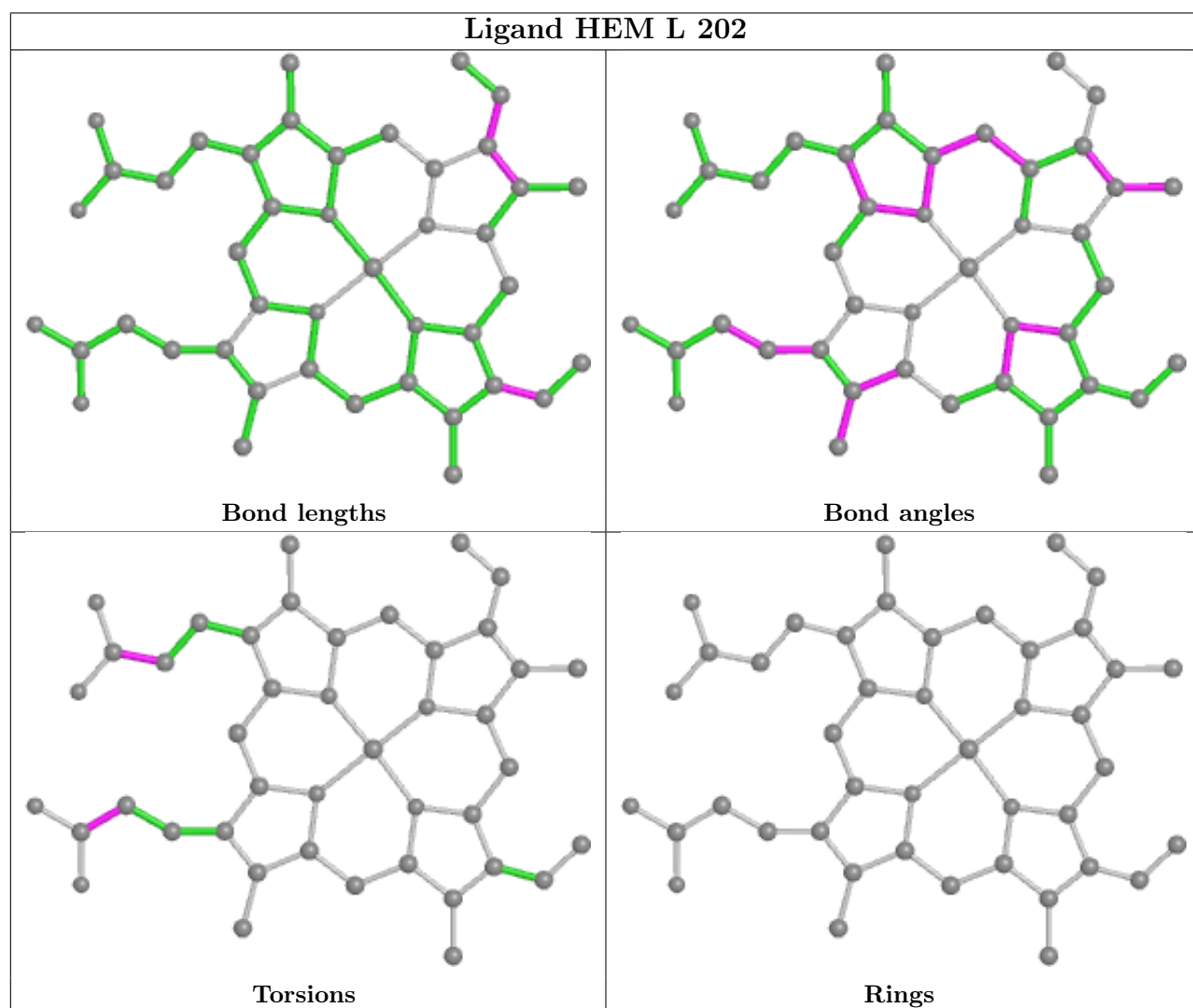
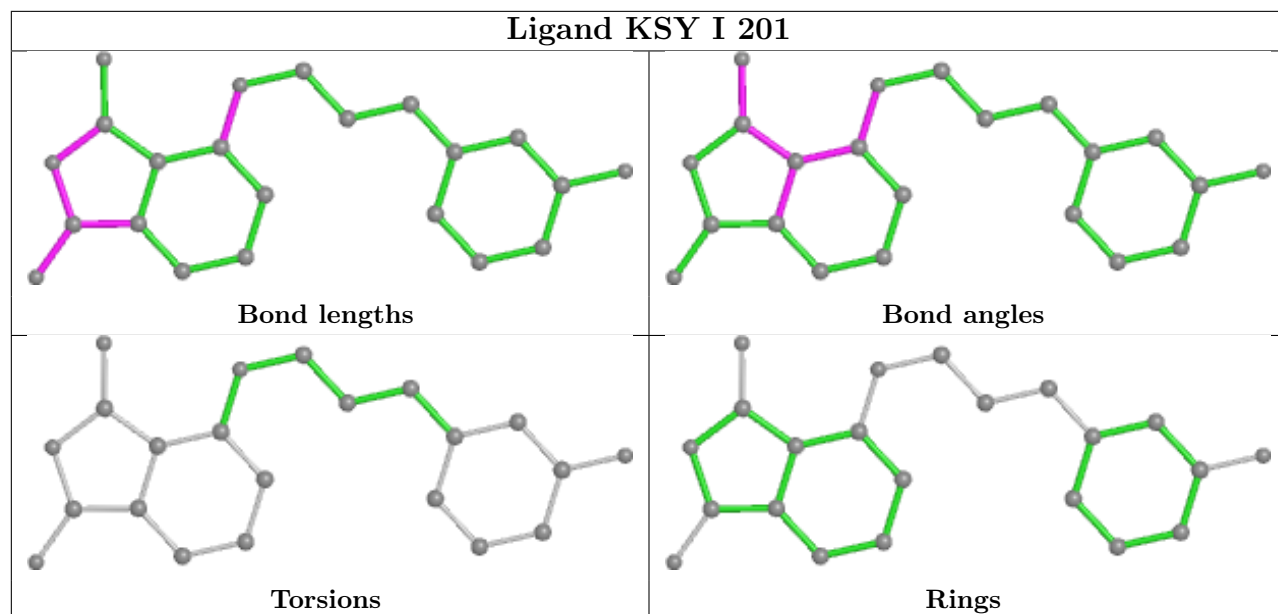
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

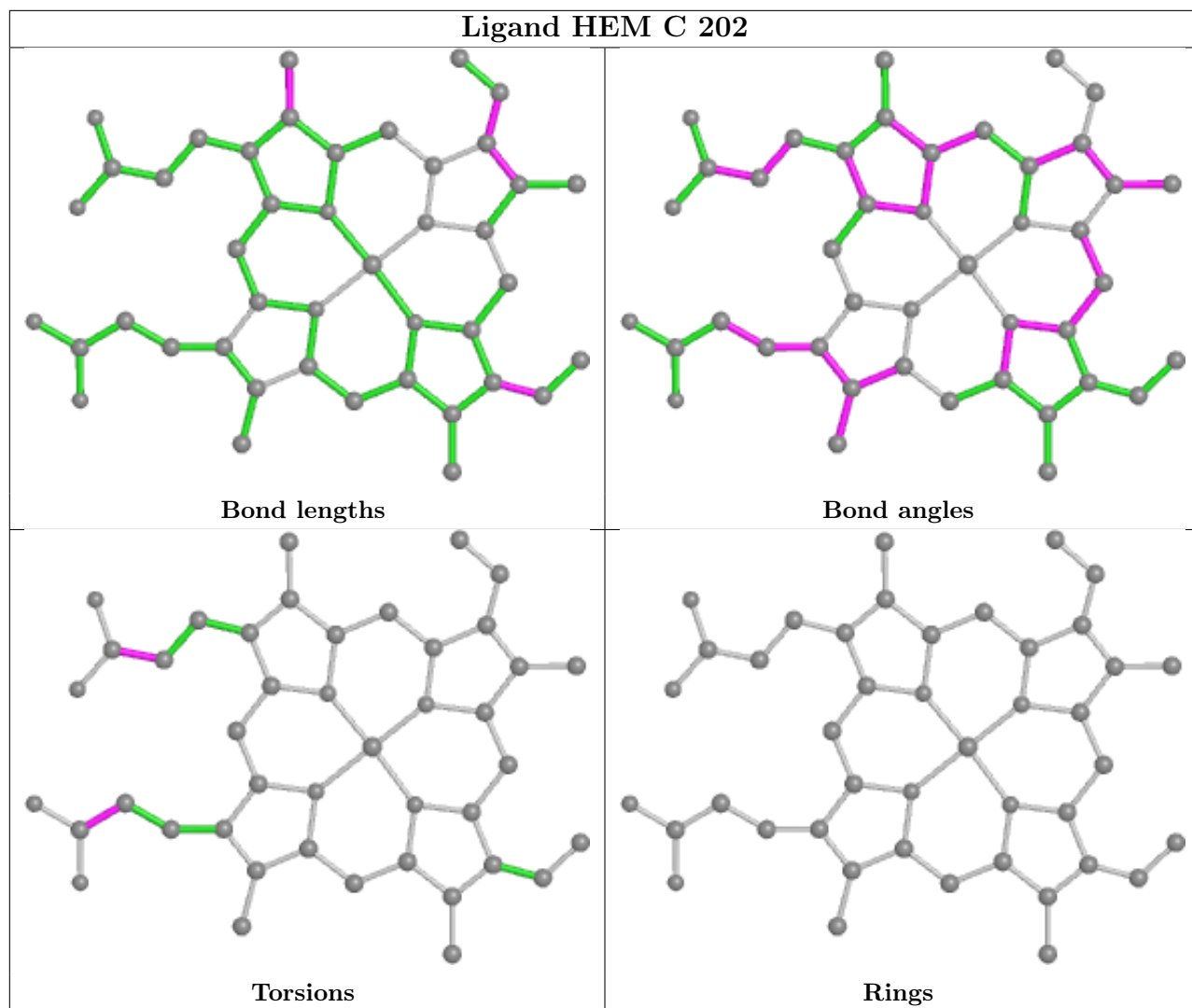


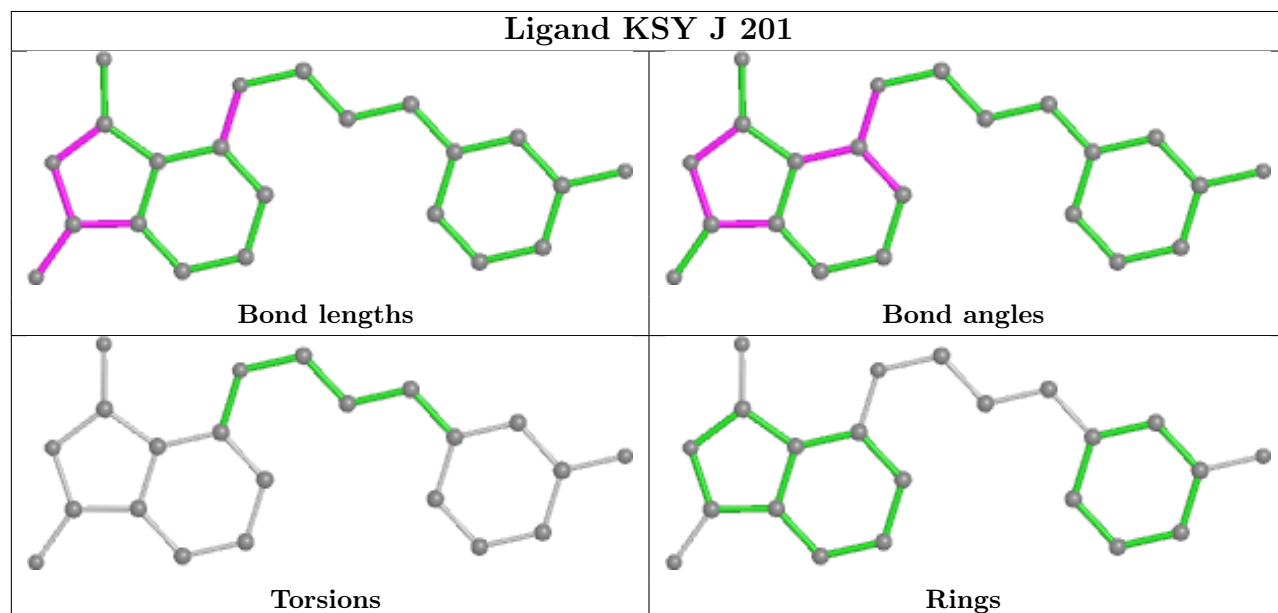
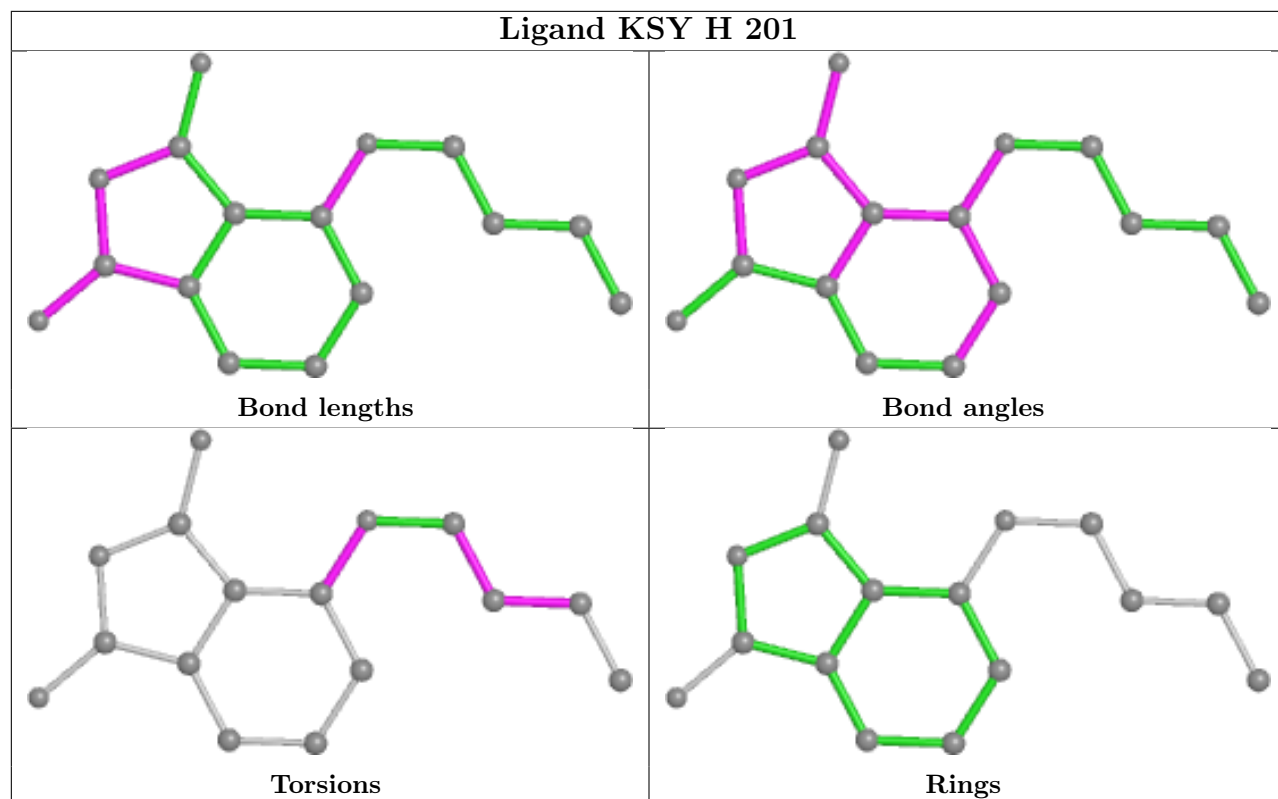


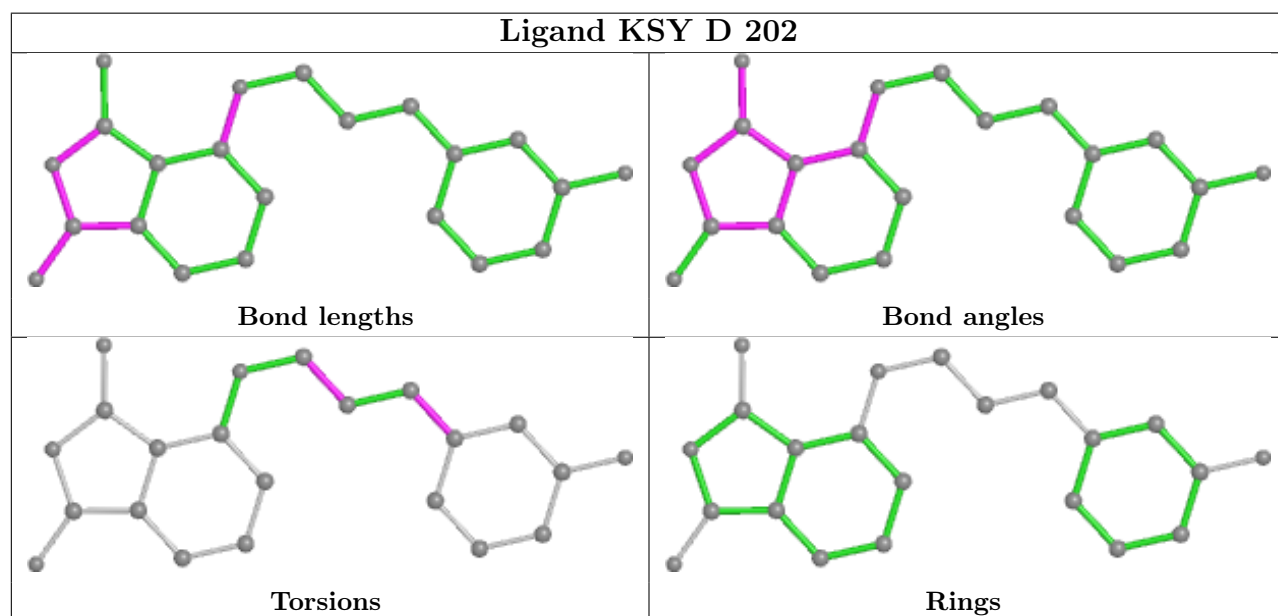
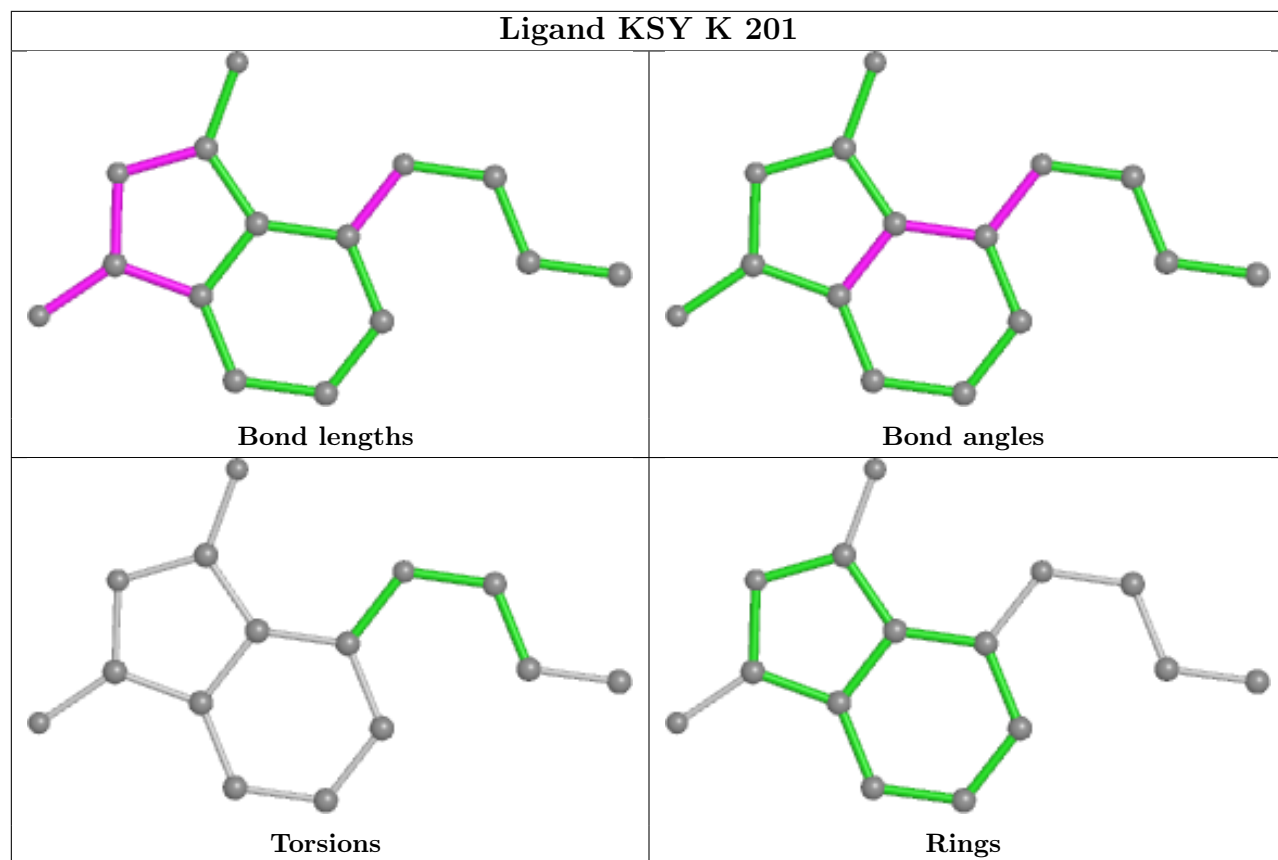


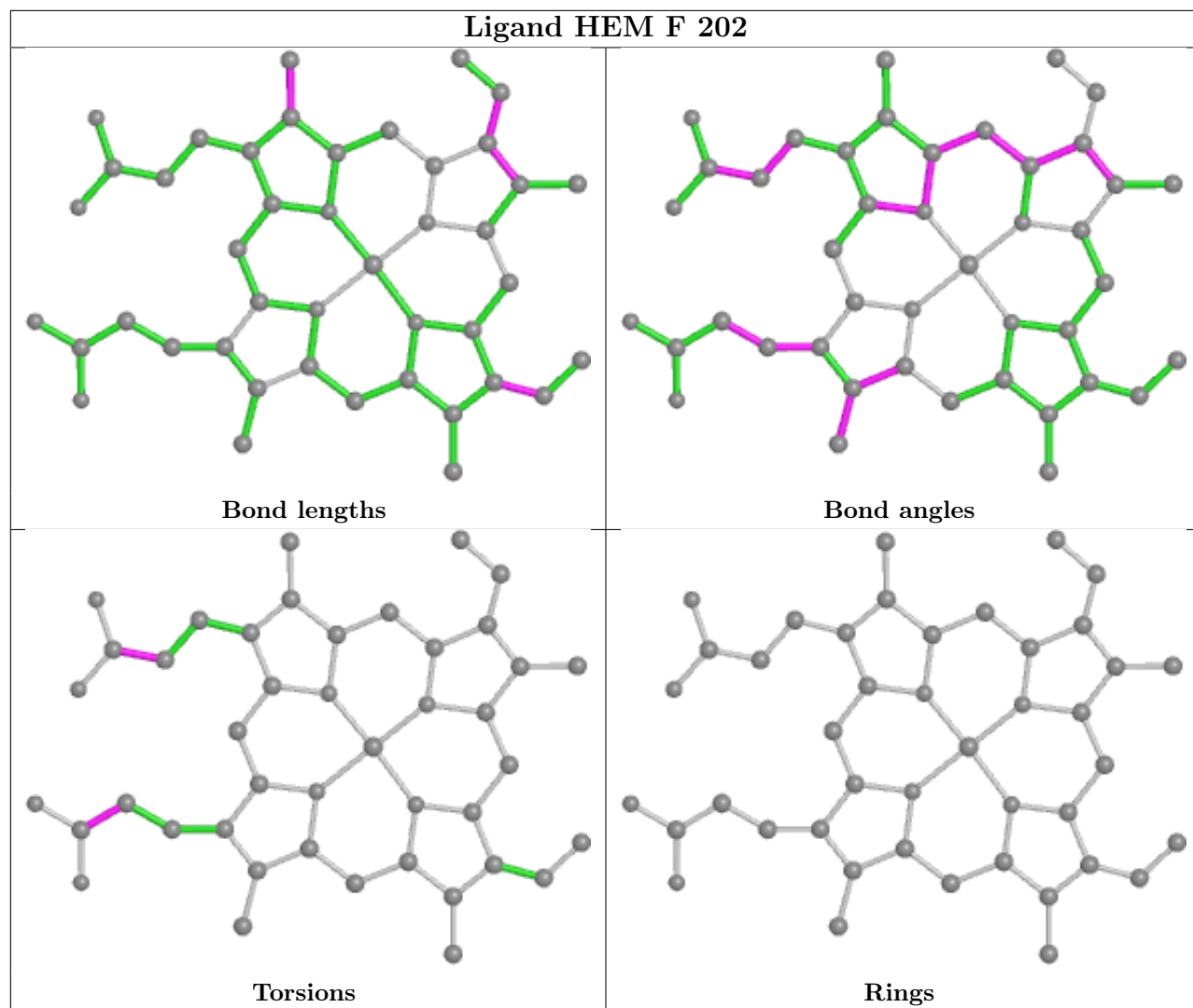


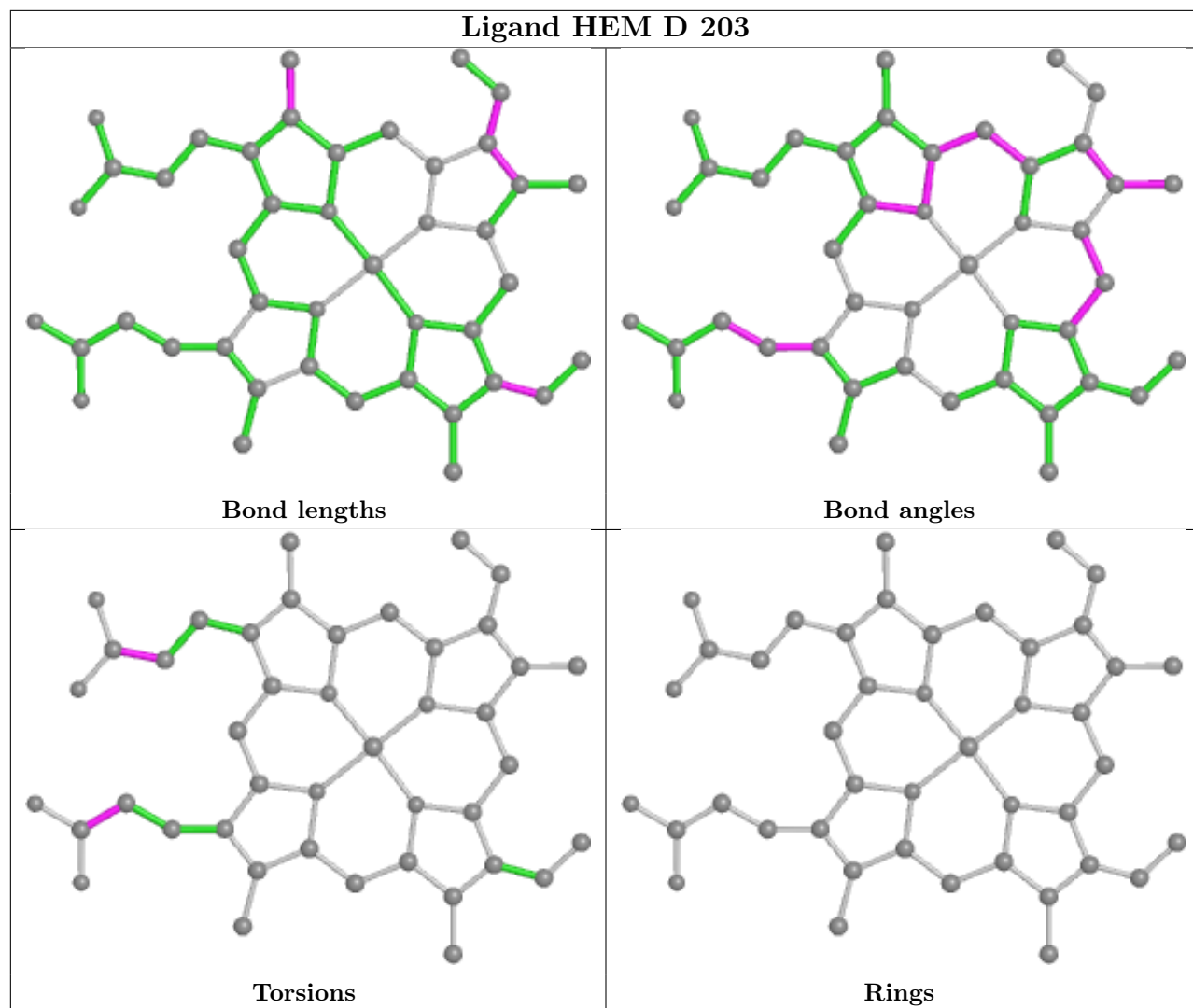


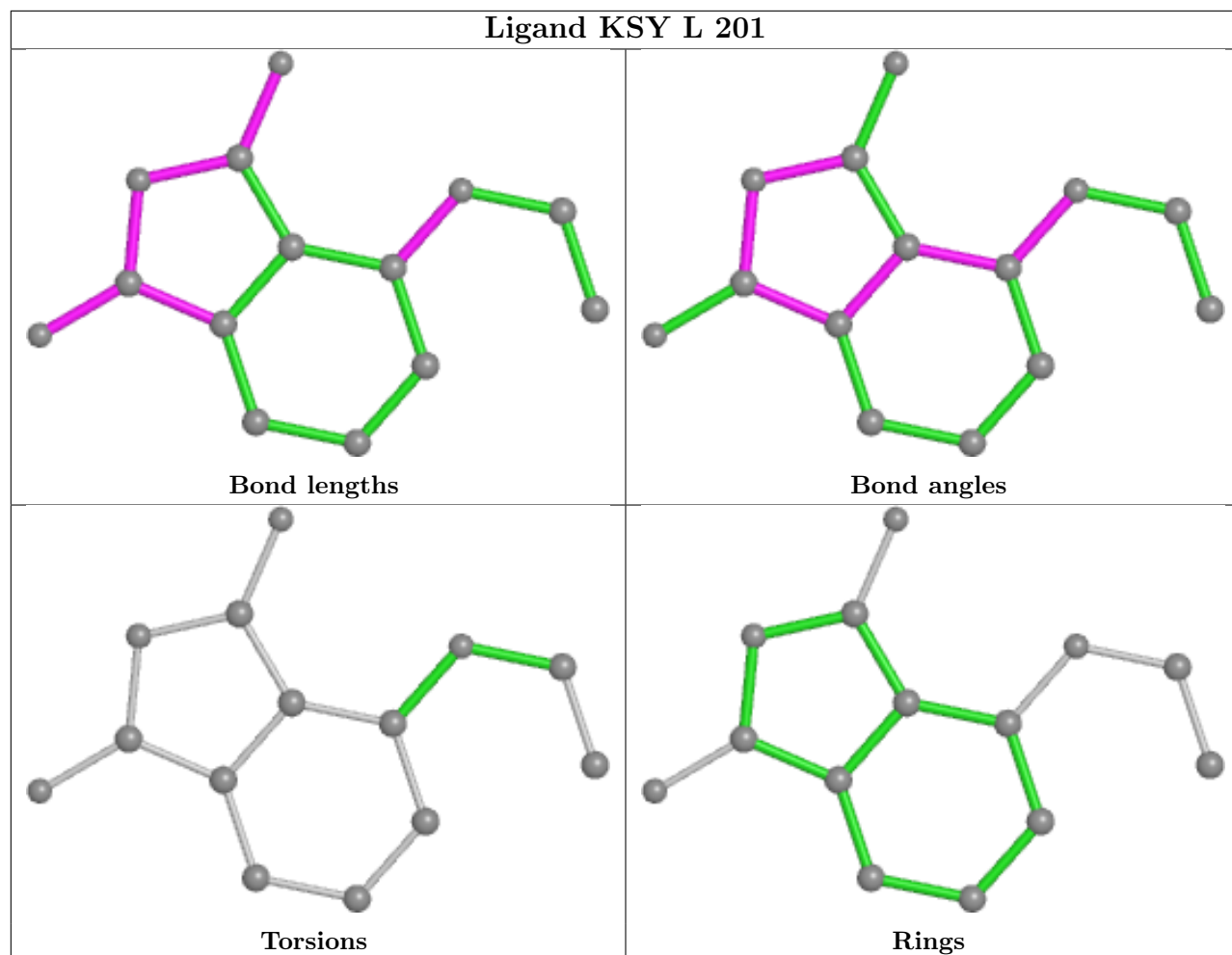


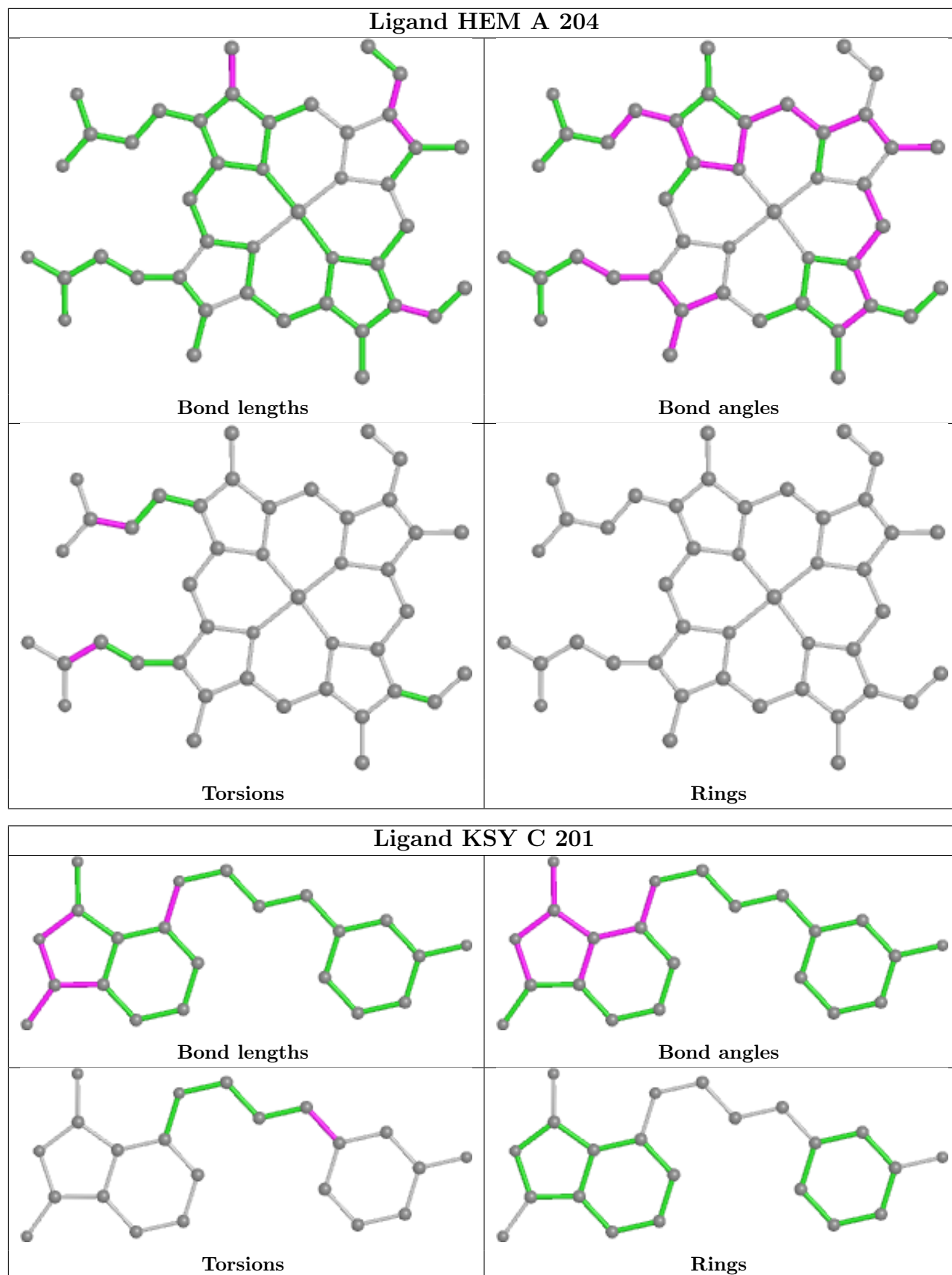


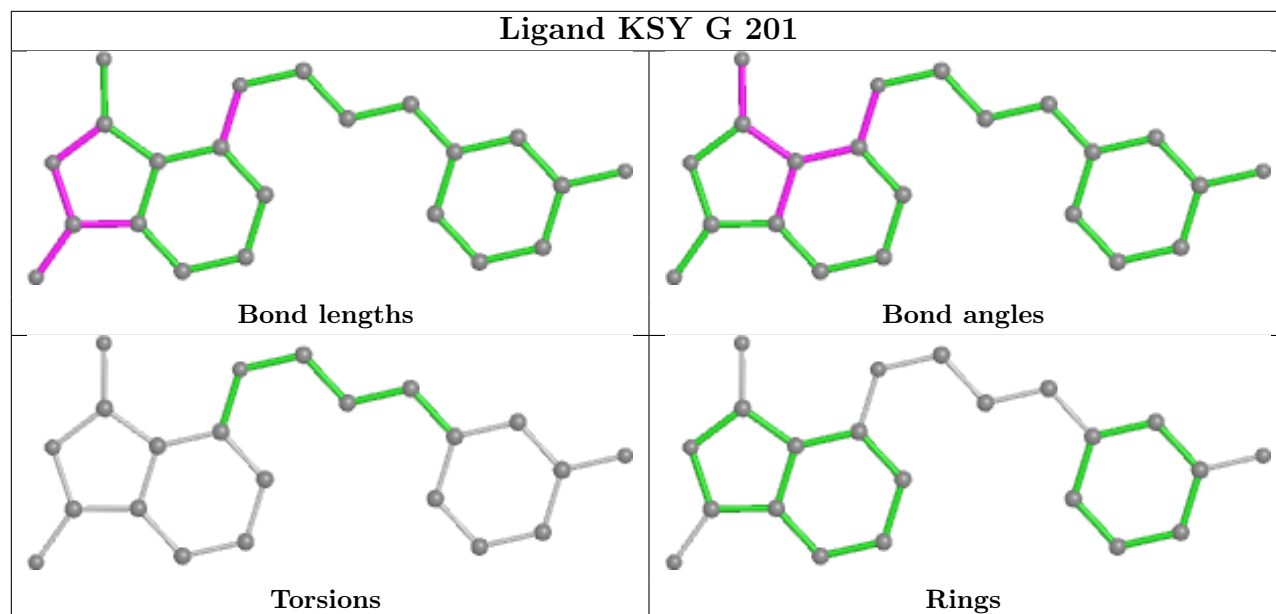












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.