



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:47 AM EDT

PDB ID : 6NH3  
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with (S)-6-(3-fluoro-5-(2-(pyrrolidin-2-yl)ethyl)phenethyl)-4-methylpyridin-2-amine  
Authors : Chreifi, G.; Li, H.; Poulos, T.L.  
Deposited on : 2018-12-21  
Resolution : 2.01 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **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 2.01 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](#)

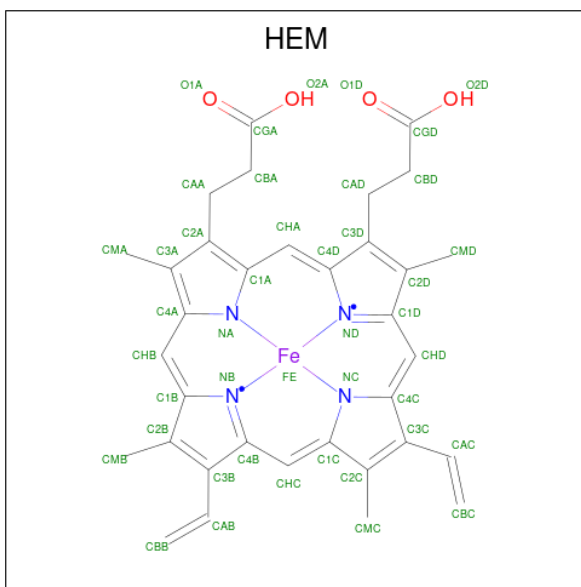
There are 9 unique types of molecules in this entry. The entry contains 13985 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endothelial nitric oxide synthase splice variant eNOS13A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	Total 3237	C 2062	N 570	O 589	S 16	0	2	0
1	B	402	Total 3221	C 2051	N 566	O 587	S 17	0	3	0
1	C	401	Total 3203	C 2040	N 563	O 584	S 16	0	1	0
1	D	402	Total 3221	C 2051	N 566	O 587	S 17	0	3	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



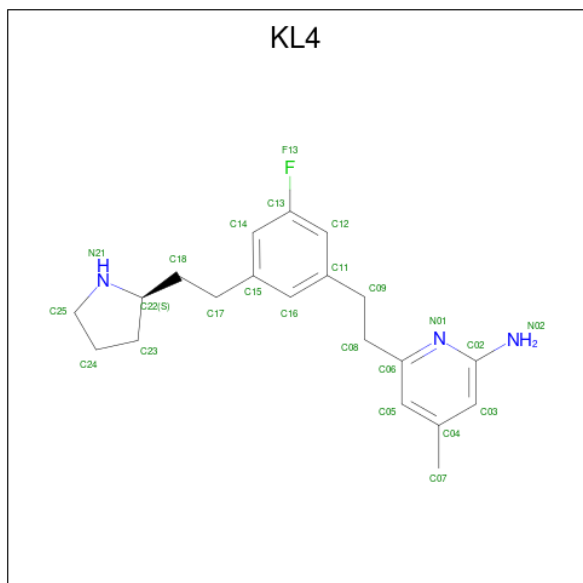
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

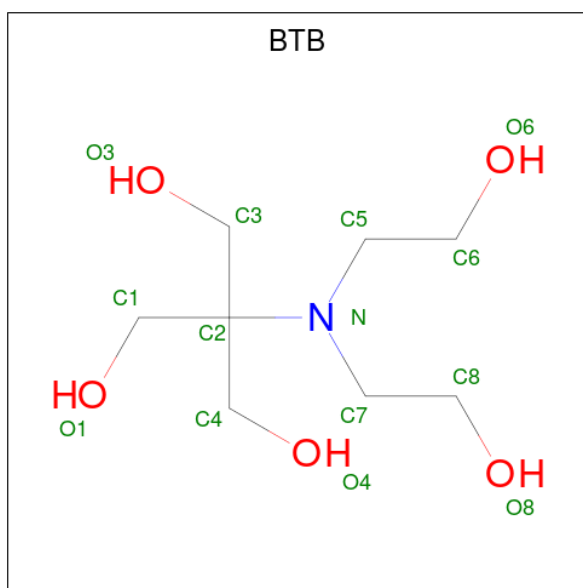
- Molecule 3 is 6-[2-(3-fluoro-5-{2-[(2S)-pyrrolidin-2-yl]ethyl}phenyl)ethyl]-4-methylpyridin-2-amine (three-letter code: KL4) (formula: C<sub>20</sub>H<sub>26</sub>FN<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			24	20	1	3		
3	A	1	Total	C	F	N	0	0
			24	20	1	3		
3	B	1	Total	C	F	N	0	0
			24	20	1	3		
3	B	1	Total	C	F	N	0	0
			24	20	1	3		
3	C	1	Total	C	F	N	0	0
			24	20	1	3		
3	C	1	Total	C	F	N	0	0
			24	20	1	3		
3	C	1	Total	C	F	N	0	0
			24	20	1	3		
3	D	1	Total	C	F	N	0	0
			24	20	1	3		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN

E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).

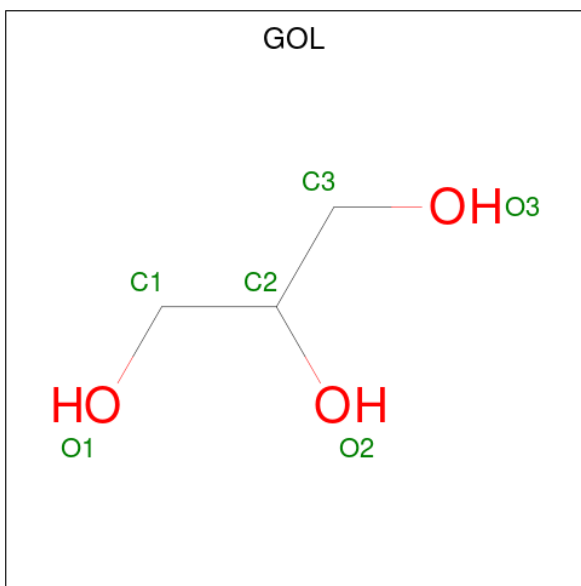


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Zn	0	0
			3	3		
5	C	3	Total	Zn	0	0
			3	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			6	3 3		
6	C	1	Total	C O	0	0
			6	3 3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Gd	0	0
			1	1		
8	B	1	Total	Gd	0	0
			1	1		
8	C	1	Total	Gd	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total 1	O Gd 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	93	Total 93	O 93	0	0
9	B	164	Total 164	O 164	0	0
9	C	126	Total 126	O 126	0	0
9	D	204	Total 204	O 204	0	0

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

### 3 Data and refinement statistics i

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.47Å 153.09Å 109.15Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	88.87 – 2.01	Depositor
% Data completeness (in resolution range)	98.4 (88.87-2.01)	Depositor
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.02Å)	Xtrriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, $R_{free}$	0.206 , 0.257	Depositor
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.747	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.087 for h,-k,-l	Xtrriage
Total number of atoms	13985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 37 ligands modelled in this entry, 14 are monoatomic - leaving 23 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
2	HEM	B	802	1	41,50,50	1.51	7 (17%)	45,82,82	1.83	12 (26%)
2	HEM	D	501	1	41,50,50	1.61	7 (17%)	45,82,82	1.75	13 (28%)
2	HEM	C	501	1	41,50,50	1.66	8 (19%)	45,82,82	1.76	11 (24%)
4	BTB	C	505	-	13,13,13	0.38	0	7,16,16	0.43	0
2	HEM	A	501	1	41,50,50	1.51	6 (14%)	45,82,82	1.61	11 (24%)
3	KL4	A	509	-	25,26,26	1.21	3 (12%)	32,35,35	1.27	4 (12%)
3	KL4	C	503	-	25,26,26	1.20	3 (12%)	32,35,35	1.36	4 (12%)
4	BTB	A	504	-	13,13,13	0.40	0	7,16,16	0.61	0
4	BTB	B	805	-	13,13,13	0.42	0	7,16,16	0.65	0
3	KL4	C	502	-	25,26,26	1.19	3 (12%)	32,35,35	1.55	6 (18%)
6	GOL	A	506	-	5,5,5	0.34	0	5,5,5	0.40	0
3	KL4	C	511	-	25,26,26	1.19	3 (12%)	32,35,35	1.39	4 (12%)
4	BTB	B	804	8	13,13,13	0.52	0	7,16,16	0.72	0
6	GOL	C	507	-	5,5,5	0.39	0	5,5,5	0.34	0
4	BTB	D	503	8	13,13,13	0.43	0	7,16,16	0.57	0
4	BTB	D	504	-	13,13,13	0.50	0	7,16,16	0.68	0
4	BTB	B	808	-	13,13,13	0.83	1 (7%)	7,16,16	0.98	1 (14%)
3	KL4	B	801	-	25,26,26	1.22	3 (12%)	32,35,35	1.32	4 (12%)
4	BTB	A	503	-	13,13,13	0.39	0	7,16,16	0.52	0
3	KL4	D	502	-	25,26,26	1.29	3 (12%)	32,35,35	1.63	8 (25%)
4	BTB	C	504	8	13,13,13	0.41	0	7,16,16	0.51	0
3	KL4	B	803	-	25,26,26	1.23	3 (12%)	32,35,35	1.85	8 (25%)
3	KL4	A	502	-	25,26,26	1.22	3 (12%)	32,35,35	1.52	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
2	HEM	B	802	1	-	4/12/54/54	-
2	HEM	D	501	1	-	2/12/54/54	-
2	HEM	C	501	1	-	6/12/54/54	-
4	BTB	C	505	-	-	6/21/21/21	-
2	HEM	A	501	1	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KL4	A	509	-	-	2/10/17/17	0/3/3/3
3	KL4	C	503	-	-	1/10/17/17	0/3/3/3
4	BTB	A	504	-	-	8/21/21/21	-
4	BTB	B	805	-	-	7/21/21/21	-
3	KL4	C	502	-	-	4/10/17/17	0/3/3/3
6	GOL	A	506	-	-	4/4/4/4	-
3	KL4	C	511	-	-	3/10/17/17	0/3/3/3
4	BTB	B	804	8	-	4/21/21/21	-
6	GOL	C	507	-	-	4/4/4/4	-
4	BTB	D	503	8	-	7/21/21/21	-
4	BTB	D	504	-	-	11/21/21/21	-
4	BTB	B	808	-	-	7/21/21/21	-
3	KL4	B	801	-	-	3/10/17/17	0/3/3/3
4	BTB	A	503	-	-	11/21/21/21	-
3	KL4	D	502	-	-	4/10/17/17	0/3/3/3
4	BTB	C	504	8	-	7/21/21/21	-
3	KL4	B	803	-	-	2/10/17/17	0/3/3/3
3	KL4	A	502	-	-	3/10/17/17	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3C-C2C	-4.13	1.34	1.40
2	B	802	HEM	C3C-CAC	4.02	1.56	1.47
2	C	501	HEM	C3C-CAC	3.99	1.56	1.47
3	D	502	KL4	C25-N21	-3.80	1.35	1.49
2	D	501	HEM	C3C-CAC	3.76	1.55	1.47
3	A	502	KL4	C25-N21	-3.73	1.35	1.49
3	B	803	KL4	C25-N21	-3.72	1.35	1.49
2	A	501	HEM	C3C-C2C	-3.67	1.35	1.40
2	A	501	HEM	C3C-CAC	3.63	1.55	1.47
3	C	502	KL4	C25-N21	-3.62	1.36	1.49
3	A	509	KL4	C25-N21	-3.58	1.36	1.49
3	B	801	KL4	C25-N21	-3.58	1.36	1.49
3	C	511	KL4	C25-N21	-3.57	1.36	1.49
3	C	503	KL4	C25-N21	-3.56	1.36	1.49
2	C	501	HEM	FE-NB	3.38	2.13	1.96
2	C	501	HEM	CAB-C3B	3.38	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	KL4	C24-C23	-3.31	1.38	1.51
2	C	501	HEM	C3C-C2C	-3.29	1.35	1.40
3	C	502	KL4	C24-C23	-3.23	1.38	1.51
2	D	501	HEM	CAA-C2A	3.23	1.56	1.52
2	D	501	HEM	FE-NB	3.22	2.12	1.96
3	B	803	KL4	C24-C23	-3.21	1.38	1.51
3	A	502	KL4	C24-C23	-3.21	1.38	1.51
3	C	511	KL4	C24-C23	-3.19	1.38	1.51
3	C	503	KL4	C24-C23	-3.14	1.38	1.51
3	A	509	KL4	C24-C23	-3.06	1.39	1.51
3	B	801	KL4	C24-C23	-3.05	1.39	1.51
2	A	501	HEM	CAA-C2A	3.04	1.56	1.52
2	B	802	HEM	C3C-C2C	-3.03	1.36	1.40
2	C	501	HEM	FE-ND	2.94	2.11	1.96
2	A	501	HEM	CAB-C3B	2.84	1.55	1.47
2	D	501	HEM	CAB-C3B	2.79	1.55	1.47
2	C	501	HEM	CAA-C2A	2.76	1.56	1.52
2	B	802	HEM	CMB-C2B	2.75	1.56	1.50
2	B	802	HEM	CAB-C3B	2.71	1.54	1.47
2	A	501	HEM	FE-NB	2.58	2.09	1.96
3	A	502	KL4	C24-C25	-2.57	1.38	1.51
3	D	502	KL4	C24-C25	-2.52	1.38	1.51
3	B	803	KL4	C24-C25	-2.50	1.38	1.51
2	D	501	HEM	CMD-C2D	2.49	1.56	1.50
2	D	501	HEM	CMB-C2B	2.49	1.56	1.50
3	C	502	KL4	C24-C25	-2.48	1.39	1.51
3	C	503	KL4	C24-C25	-2.45	1.39	1.51
3	A	509	KL4	C24-C25	-2.43	1.39	1.51
3	B	801	KL4	C24-C25	-2.43	1.39	1.51
2	B	802	HEM	CAA-C2A	2.41	1.55	1.52
3	C	511	KL4	C24-C25	-2.39	1.39	1.51
2	B	802	HEM	FE-NB	2.32	2.08	1.96
2	C	501	HEM	CMB-C2B	2.15	1.55	1.50
2	C	501	HEM	CMD-C2D	2.10	1.55	1.50
4	B	808	BTB	C1-C2	-2.06	1.50	1.53
2	B	802	HEM	FE-ND	2.04	2.06	1.96
2	A	501	HEM	C3B-C2B	-2.02	1.33	1.37

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CMA-C3A-C4A	-5.33	120.27	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	KL4	C02-N01-C06	4.96	121.86	118.10
2	B	802	HEM	CMA-C3A-C4A	-4.91	120.92	128.46
3	A	502	KL4	C02-N01-C06	4.77	121.72	118.10
2	D	501	HEM	CMA-C3A-C4A	-4.67	121.29	128.46
3	B	803	KL4	C02-N01-C06	4.40	121.44	118.10
3	B	801	KL4	C02-N01-C06	3.84	121.01	118.10
3	C	502	KL4	C02-N01-C06	3.75	120.94	118.10
3	B	803	KL4	C14-C13-C12	-3.70	118.85	123.52
2	B	802	HEM	C1B-NB-C4B	3.65	108.84	105.07
2	A	501	HEM	CMA-C3A-C4A	-3.64	122.88	128.46
3	B	803	KL4	C04-C05-C06	-3.55	118.00	120.32
2	C	501	HEM	C4B-CHC-C1C	3.50	127.18	122.56
3	C	503	KL4	C02-N01-C06	3.49	120.74	118.10
2	C	501	HEM	CMA-C3A-C2A	3.48	131.51	124.94
3	C	511	KL4	C09-C08-C06	-3.39	105.40	112.99
3	B	803	KL4	C18-C17-C15	-3.34	101.56	113.18
3	A	509	KL4	C02-N01-C06	3.25	120.56	118.10
2	B	802	HEM	CMA-C3A-C2A	3.24	131.04	124.94
2	D	501	HEM	CBA-CAA-C2A	3.22	118.11	112.62
2	B	802	HEM	CHC-C4B-C3B	3.12	129.34	124.57
2	B	802	HEM	CMC-C2C-C3C	3.07	130.42	124.68
3	C	502	KL4	C08-C06-N01	3.06	120.51	115.95
3	C	502	KL4	C18-C17-C15	-2.99	102.78	113.18
3	C	503	KL4	C14-C13-C12	-2.97	119.76	123.52
2	D	501	HEM	C4B-CHC-C1C	2.94	126.44	122.56
3	C	511	KL4	C02-N01-C06	2.94	120.33	118.10
3	C	511	KL4	C14-C13-C12	-2.91	119.84	123.52
2	B	802	HEM	C4B-CHC-C1C	2.90	126.38	122.56
2	C	501	HEM	C1B-NB-C4B	2.88	108.05	105.07
2	A	501	HEM	C3B-C2B-C1B	2.85	108.60	106.49
2	C	501	HEM	CBA-CAA-C2A	2.81	117.42	112.62
3	D	502	KL4	C14-C13-C12	-2.79	120.00	123.52
3	A	502	KL4	C14-C13-C12	-2.78	120.00	123.52
3	A	502	KL4	C05-C06-N01	-2.77	119.97	122.90
2	D	501	HEM	CMC-C2C-C3C	2.74	129.80	124.68
2	A	501	HEM	C4D-ND-C1D	2.68	107.84	105.07
2	B	802	HEM	C4D-ND-C1D	2.64	107.81	105.07
3	A	509	KL4	C05-C06-N01	-2.64	120.10	122.90
3	A	509	KL4	C14-C13-C12	-2.63	120.19	123.52
2	D	501	HEM	CBD-CAD-C3D	-2.63	105.31	112.63
2	A	501	HEM	CHB-C1B-NB	2.63	127.63	124.38
2	D	501	HEM	CMA-C3A-C2A	2.63	129.89	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C4A-C3A-C2A	2.62	108.82	107.00
2	D	501	HEM	CHC-C4B-C3B	2.61	128.56	124.57
3	B	801	KL4	C08-C06-N01	2.58	119.80	115.95
3	C	502	KL4	N02-C02-N01	2.57	120.55	116.49
3	D	502	KL4	C18-C17-C15	-2.55	104.32	113.18
2	C	501	HEM	C3D-C4D-ND	-2.54	107.34	110.17
3	B	801	KL4	C14-C13-C12	-2.54	120.31	123.52
2	C	501	HEM	CBD-CAD-C3D	-2.52	105.61	112.63
3	A	509	KL4	C08-C06-N01	2.50	119.67	115.95
2	D	501	HEM	C1B-NB-C4B	2.47	107.63	105.07
2	A	501	HEM	CHC-C4B-C3B	2.47	128.35	124.57
3	C	502	KL4	C05-C06-N01	-2.45	120.31	122.90
2	C	501	HEM	C4D-ND-C1D	2.42	107.57	105.07
2	B	802	HEM	CAA-C2A-C3A	2.41	134.17	127.25
2	A	501	HEM	C4B-CHC-C1C	2.41	125.73	122.56
3	B	803	KL4	C15-C16-C11	-2.40	118.28	121.23
3	C	503	KL4	C08-C06-N01	2.38	119.50	115.95
2	B	802	HEM	C4B-C3B-C2B	2.38	109.00	107.11
3	B	801	KL4	C05-C06-N01	-2.37	120.39	122.90
2	C	501	HEM	CHC-C4B-C3B	2.37	128.19	124.57
2	D	501	HEM	C4D-ND-C1D	2.32	107.47	105.07
3	B	803	KL4	C11-C12-C13	2.32	120.92	118.81
2	A	501	HEM	C1B-NB-C4B	2.31	107.46	105.07
2	D	501	HEM	C3D-C4D-ND	-2.29	107.61	110.17
3	D	502	KL4	C05-C06-N01	-2.29	120.47	122.90
2	D	501	HEM	CAA-C2A-C3A	2.26	133.75	127.25
2	B	802	HEM	C4C-CHD-C1D	2.26	125.54	122.56
2	A	501	HEM	CMA-C3A-C2A	2.26	129.20	124.94
3	C	503	KL4	C05-C06-N01	-2.23	120.54	122.90
3	C	511	KL4	C24-C25-N21	2.19	112.10	105.69
2	C	501	HEM	CAD-C3D-C2D	-2.19	123.80	127.88
2	A	501	HEM	C3D-C4D-ND	-2.19	107.73	110.17
3	D	502	KL4	C24-C25-N21	2.18	112.05	105.69
2	A	501	HEM	CMC-C2C-C3C	2.16	128.72	124.68
3	D	502	KL4	C11-C12-C13	2.16	120.78	118.81
2	B	802	HEM	CAA-CBA-CGA	-2.12	107.82	113.76
3	C	502	KL4	C14-C13-C12	-2.09	120.88	123.52
3	D	502	KL4	C08-C06-N01	2.06	119.02	115.95
4	B	808	BTB	O1-C1-C2	-2.05	105.83	111.44
2	D	501	HEM	C4C-CHD-C1D	2.04	125.25	122.56
3	B	803	KL4	C16-C15-C14	2.02	121.76	118.98
2	A	501	HEM	CBD-CAD-C3D	-2.02	107.01	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	KL4	C08-C09-C11	-2.02	106.18	113.28
3	D	502	KL4	F13-C13-C12	2.02	121.13	118.25
2	C	501	HEM	C3B-C2B-C1B	2.02	107.98	106.49
2	B	802	HEM	CAB-C3B-C2B	-2.01	121.97	128.60

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	B	802	HEM	C1A-C2A-CAA-CBA
2	B	802	HEM	C3A-C2A-CAA-CBA
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
2	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
3	A	502	KL4	C15-C17-C18-C22
3	A	509	KL4	C17-C18-C22-N21
3	B	801	KL4	C17-C18-C22-N21
3	B	803	KL4	C17-C18-C22-C23
3	B	803	KL4	C17-C18-C22-N21
3	C	502	KL4	C17-C18-C22-C23
3	C	502	KL4	C17-C18-C22-N21
3	C	511	KL4	C17-C18-C22-N21
3	D	502	KL4	C17-C18-C22-C23
3	D	502	KL4	C17-C18-C22-N21
4	A	503	BTB	C1-C2-C4-O4
4	A	503	BTB	C3-C2-C4-O4
4	A	503	BTB	N-C2-C4-O4
4	A	503	BTB	C1-C2-N-C5
4	A	503	BTB	C1-C2-N-C7
4	A	503	BTB	C3-C2-N-C5
4	A	503	BTB	C3-C2-N-C7
4	A	503	BTB	C4-C2-N-C5
4	A	503	BTB	C4-C2-N-C7
4	A	504	BTB	C1-C2-C3-O3
4	A	504	BTB	C4-C2-C3-O3
4	A	504	BTB	N-C2-C3-O3
4	A	504	BTB	C1-C2-C4-O4
4	A	504	BTB	C3-C2-C4-O4
4	A	504	BTB	N-C2-C4-O4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
4	B	804	BTB	O1-C1-C2-C3
4	B	804	BTB	O1-C1-C2-C4
4	B	804	BTB	O1-C1-C2-N
4	B	805	BTB	O1-C1-C2-C4
4	B	805	BTB	C1-C2-C4-O4
4	B	805	BTB	C3-C2-C4-O4
4	B	805	BTB	N-C2-C4-O4
4	B	808	BTB	C1-C2-C3-O3
4	B	808	BTB	C4-C2-C3-O3
4	B	808	BTB	N-C2-C3-O3
4	B	808	BTB	C1-C2-C4-O4
4	B	808	BTB	C3-C2-C4-O4
4	B	808	BTB	C8-C7-N-C5
4	C	504	BTB	O1-C1-C2-C3
4	C	504	BTB	O1-C1-C2-C4
4	C	504	BTB	O1-C1-C2-N
4	C	504	BTB	C1-C2-C4-O4
4	C	504	BTB	C3-C2-C4-O4
4	C	504	BTB	N-C2-C4-O4
4	C	505	BTB	C1-C2-C3-O3
4	C	505	BTB	C4-C2-C3-O3
4	C	505	BTB	N-C2-C3-O3
4	C	505	BTB	C1-C2-C4-O4
4	C	505	BTB	C3-C2-C4-O4
4	C	505	BTB	N-C2-C4-O4
4	D	503	BTB	O1-C1-C2-C3
4	D	503	BTB	O1-C1-C2-C4
4	D	503	BTB	O1-C1-C2-N
4	D	503	BTB	C1-C2-C4-O4
4	D	503	BTB	C3-C2-C4-O4
4	D	503	BTB	N-C2-C4-O4
4	D	503	BTB	N-C5-C6-O6
4	D	504	BTB	O1-C1-C2-C3
4	D	504	BTB	O1-C1-C2-C4
4	D	504	BTB	O1-C1-C2-N
4	D	504	BTB	C1-C2-C3-O3
4	D	504	BTB	C4-C2-C3-O3
4	D	504	BTB	C3-C2-C4-O4
4	D	504	BTB	C8-C7-N-C5
6	A	506	GOL	O1-C1-C2-C3
6	A	506	GOL	C1-C2-C3-O3
4	A	503	BTB	N-C5-C6-O6

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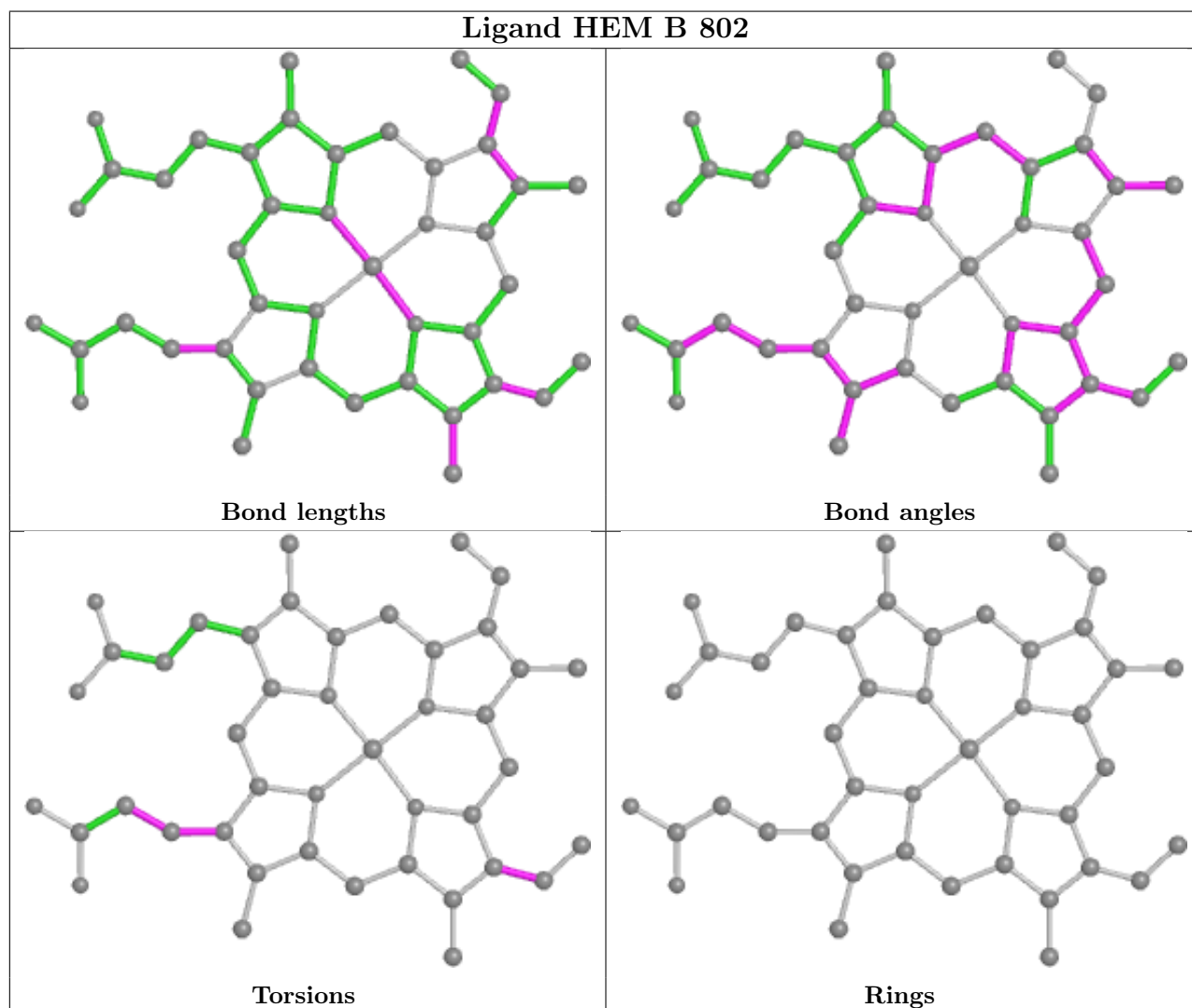
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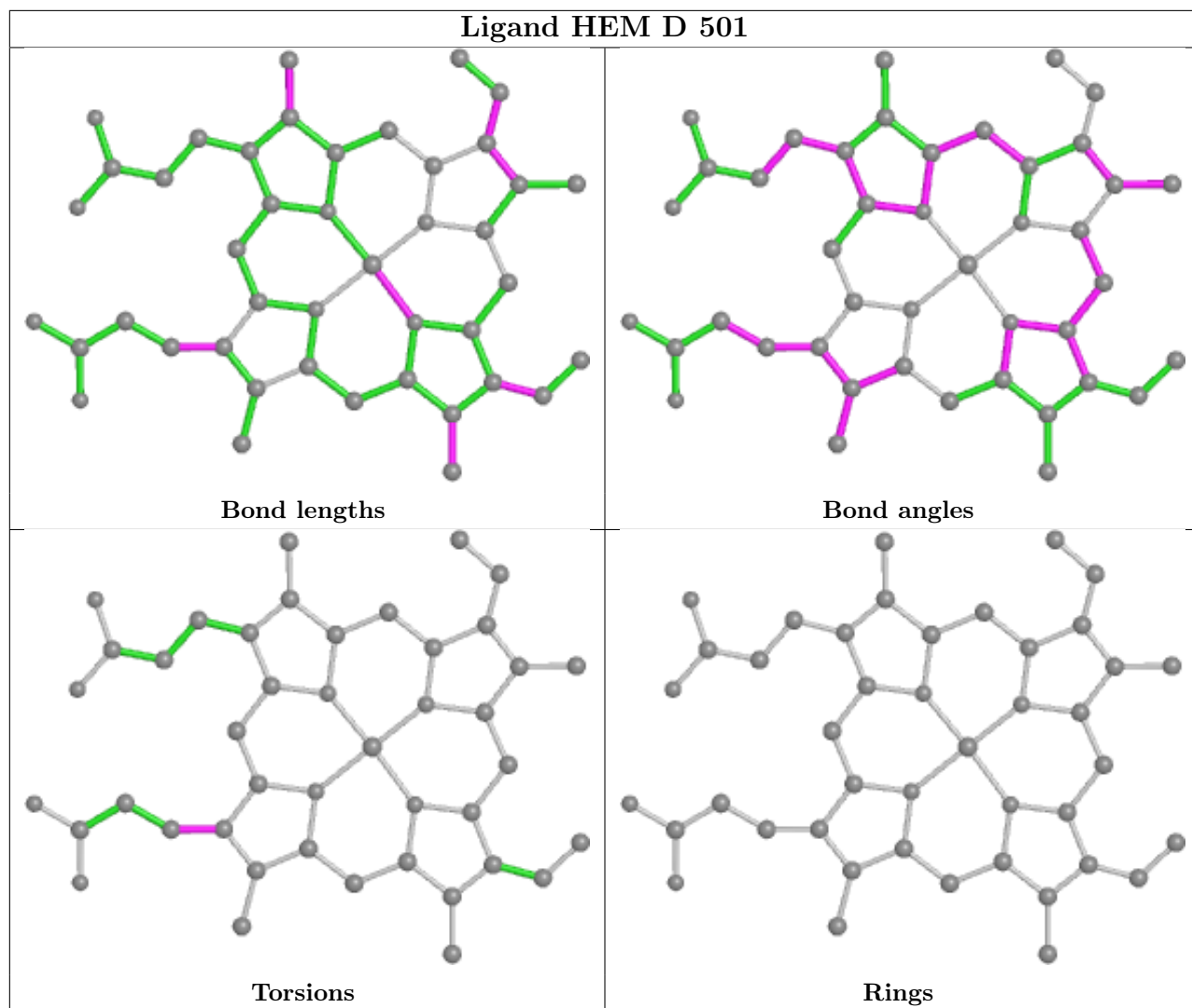
Mol	Chain	Res	Type	Atoms
4	A	503	BTB	N-C7-C8-O8
2	A	501	HEM	C2A-CAA-CBA-CGA
6	A	506	GOL	O1-C1-C2-O2
4	C	504	BTB	N-C7-C8-O8
4	D	504	BTB	N-C7-C8-O8
4	D	504	BTB	N-C5-C6-O6
6	C	507	GOL	O1-C1-C2-C3
4	A	504	BTB	N-C5-C6-O6
2	C	501	HEM	C2A-CAA-CBA-CGA
6	A	506	GOL	O2-C2-C3-O3
6	C	507	GOL	O1-C1-C2-O2
2	B	802	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	802	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
6	C	507	GOL	O2-C2-C3-O3
3	C	503	KL4	C17-C18-C22-N21
4	B	805	BTB	O1-C1-C2-C3
4	B	805	BTB	O1-C1-C2-N
4	B	808	BTB	N-C2-C4-O4
4	D	504	BTB	N-C2-C3-O3
3	D	502	KL4	C14-C15-C17-C18
3	D	502	KL4	C16-C15-C17-C18
3	B	801	KL4	C14-C15-C17-C18
4	B	805	BTB	N-C5-C6-O6
2	C	501	HEM	CAA-CBA-CGA-O2A
3	C	511	KL4	C14-C15-C17-C18
2	C	501	HEM	CAA-CBA-CGA-O1A
3	B	801	KL4	C16-C15-C17-C18
3	C	511	KL4	C16-C15-C17-C18
3	A	502	KL4	C14-C15-C17-C18
4	A	504	BTB	N-C7-C8-O8
3	A	502	KL4	C16-C15-C17-C18
3	C	502	KL4	C14-C15-C17-C18
4	B	804	BTB	N-C7-C8-O8
6	C	507	GOL	C1-C2-C3-O3
3	C	502	KL4	C16-C15-C17-C18
3	A	509	KL4	C17-C18-C22-C23
4	D	504	BTB	C1-C2-C4-O4

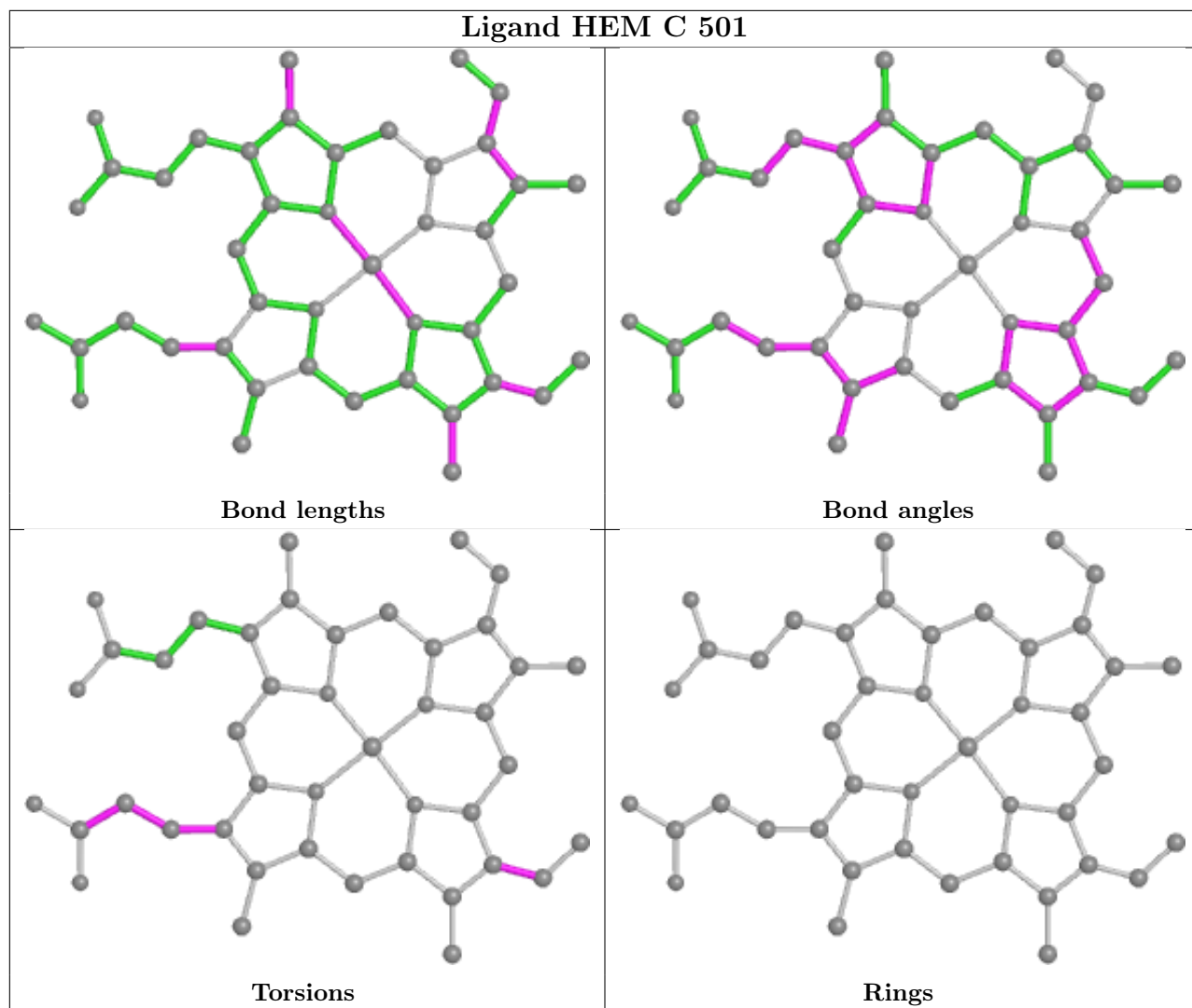
There are no ring outliers.

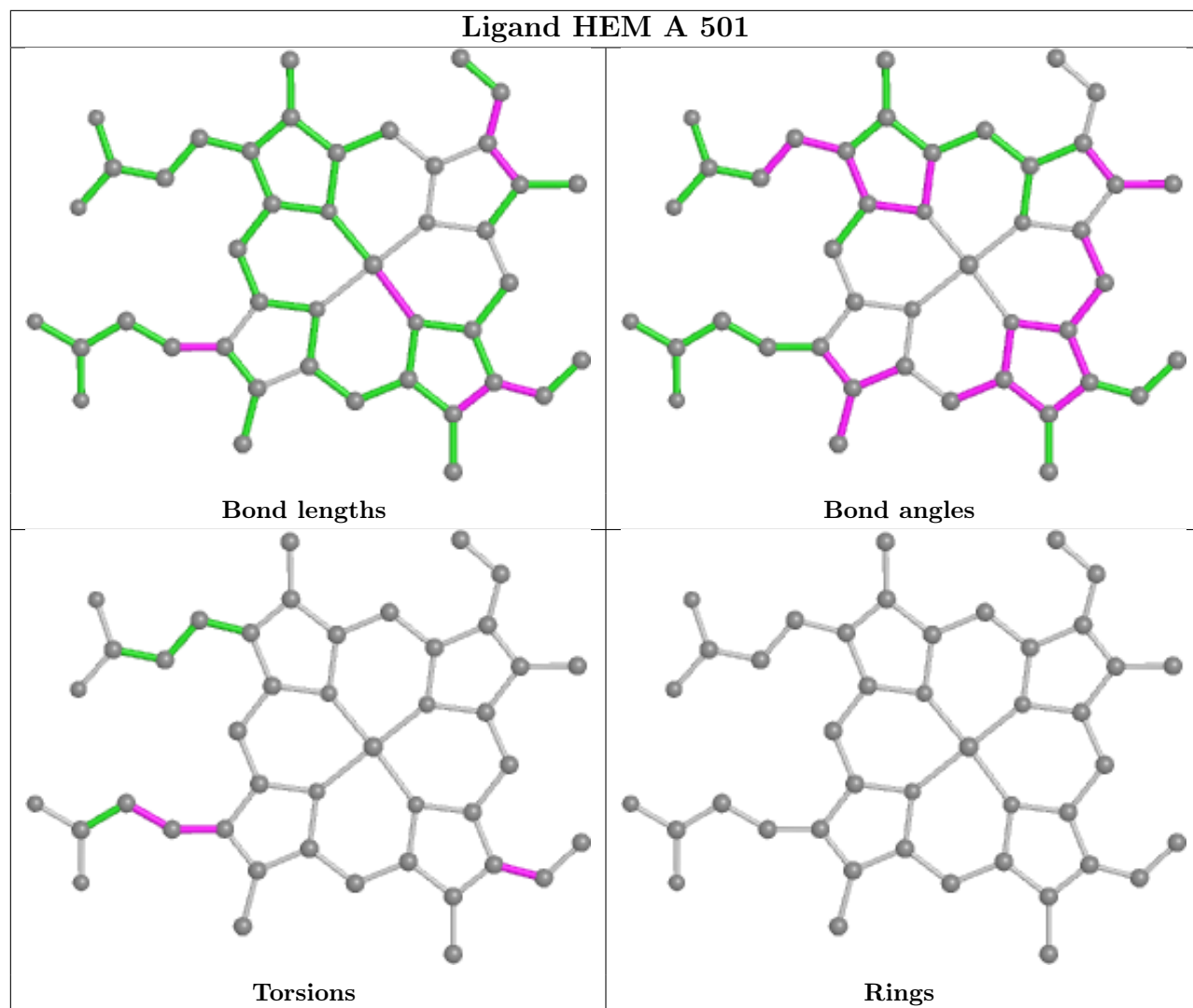
No monomer is involved in short contacts.

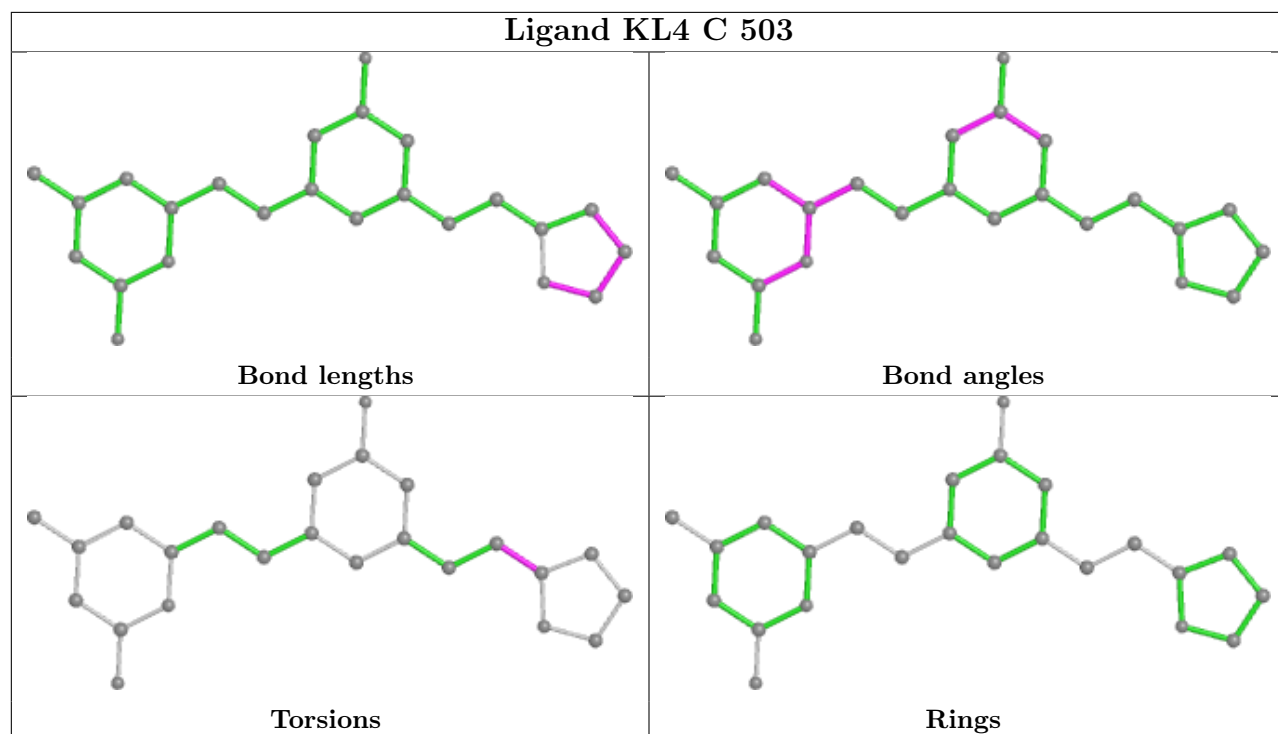
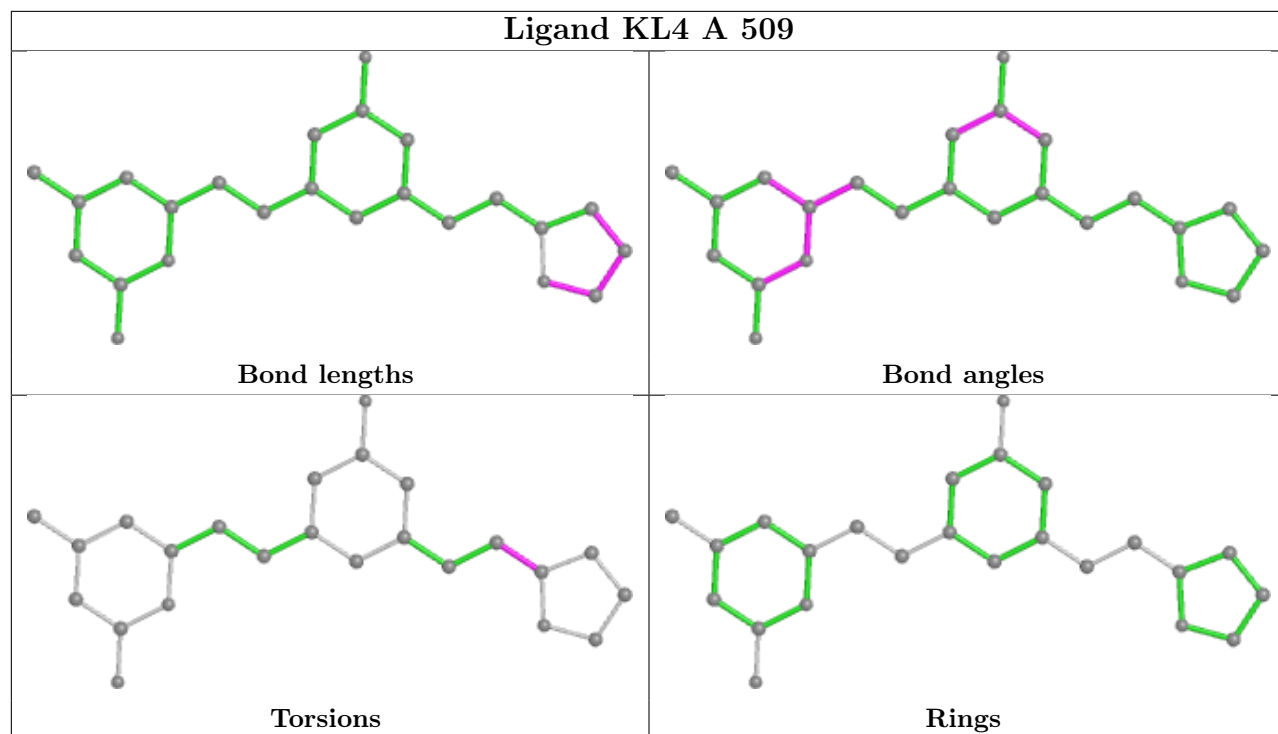
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

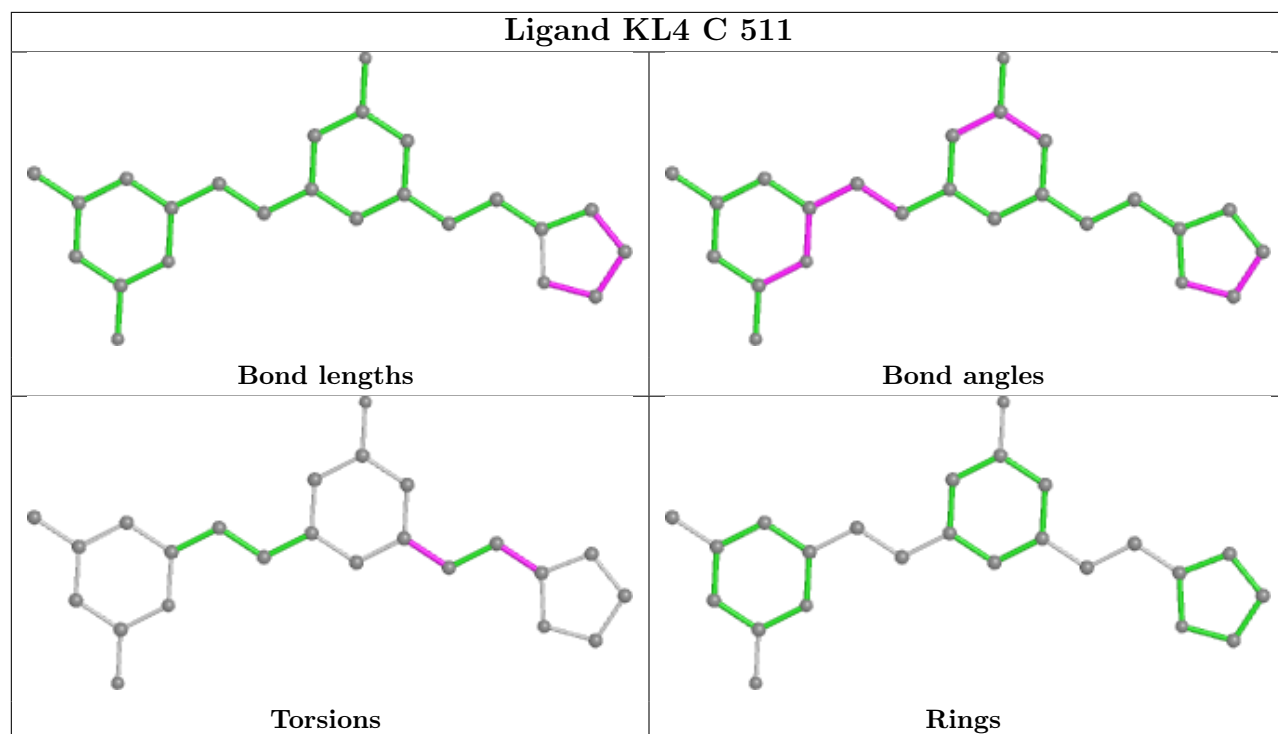
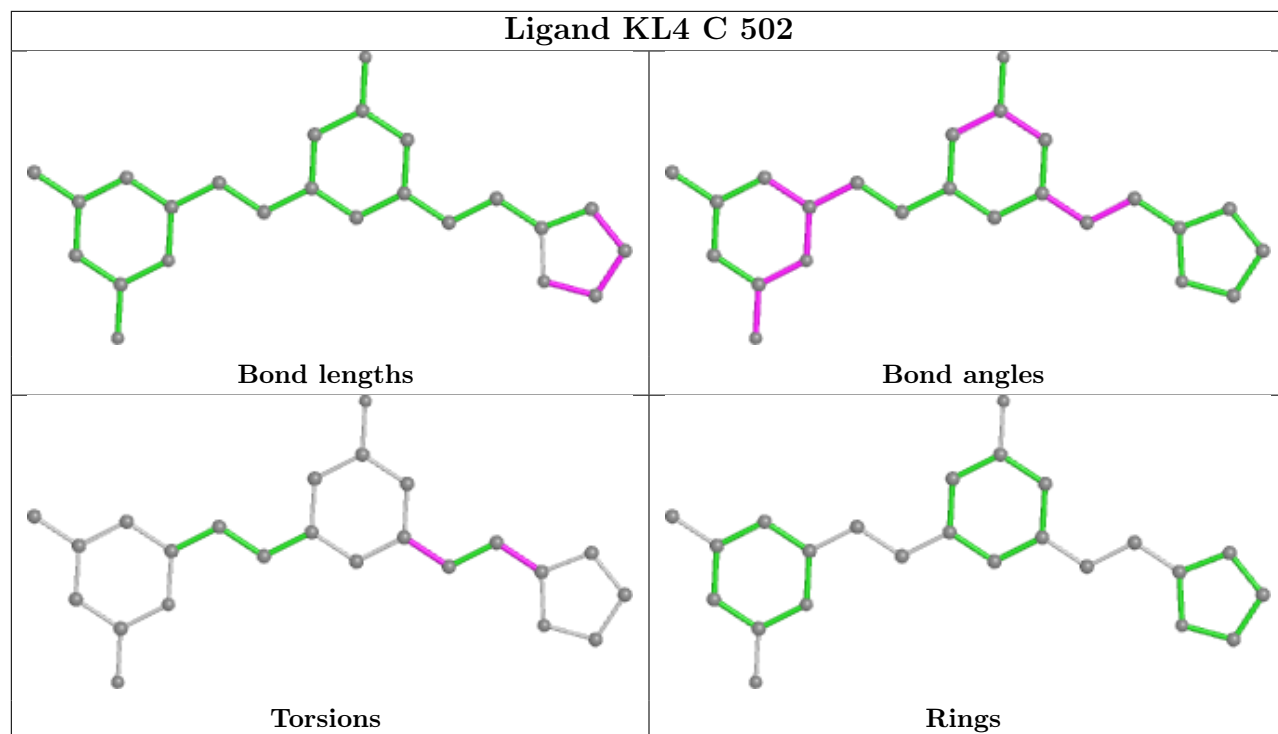


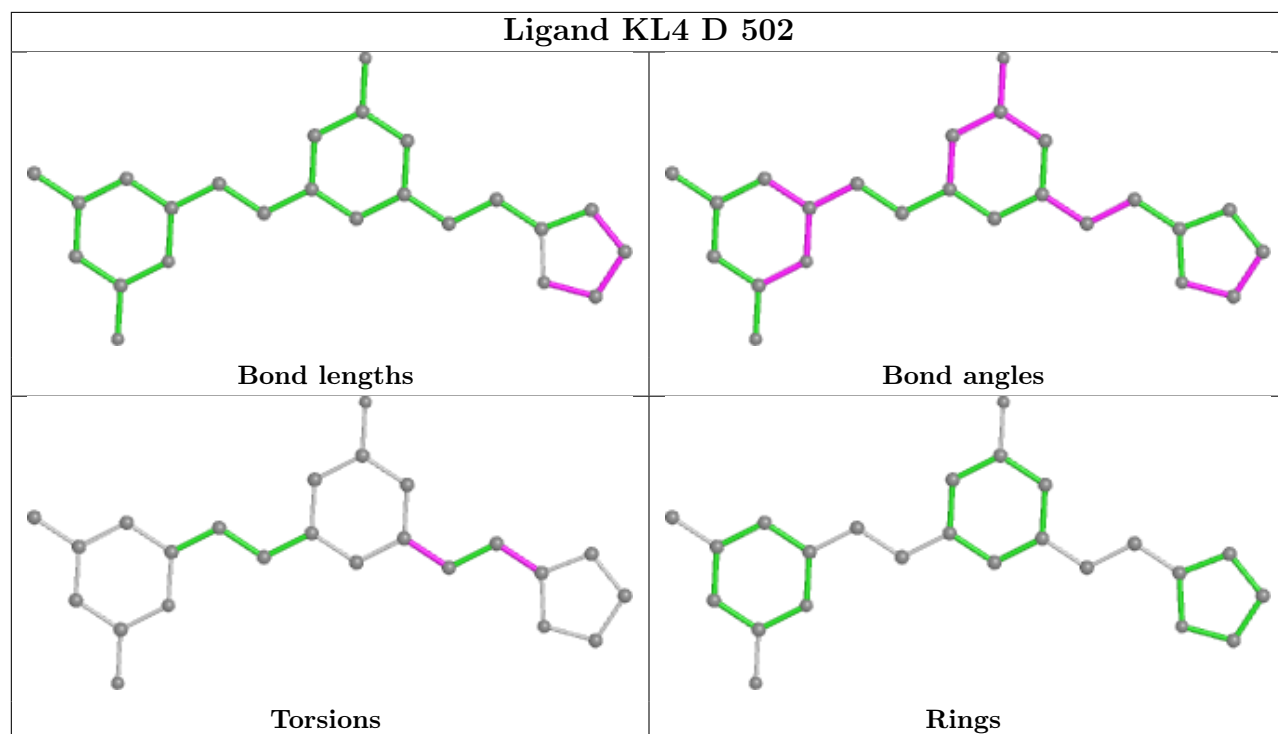
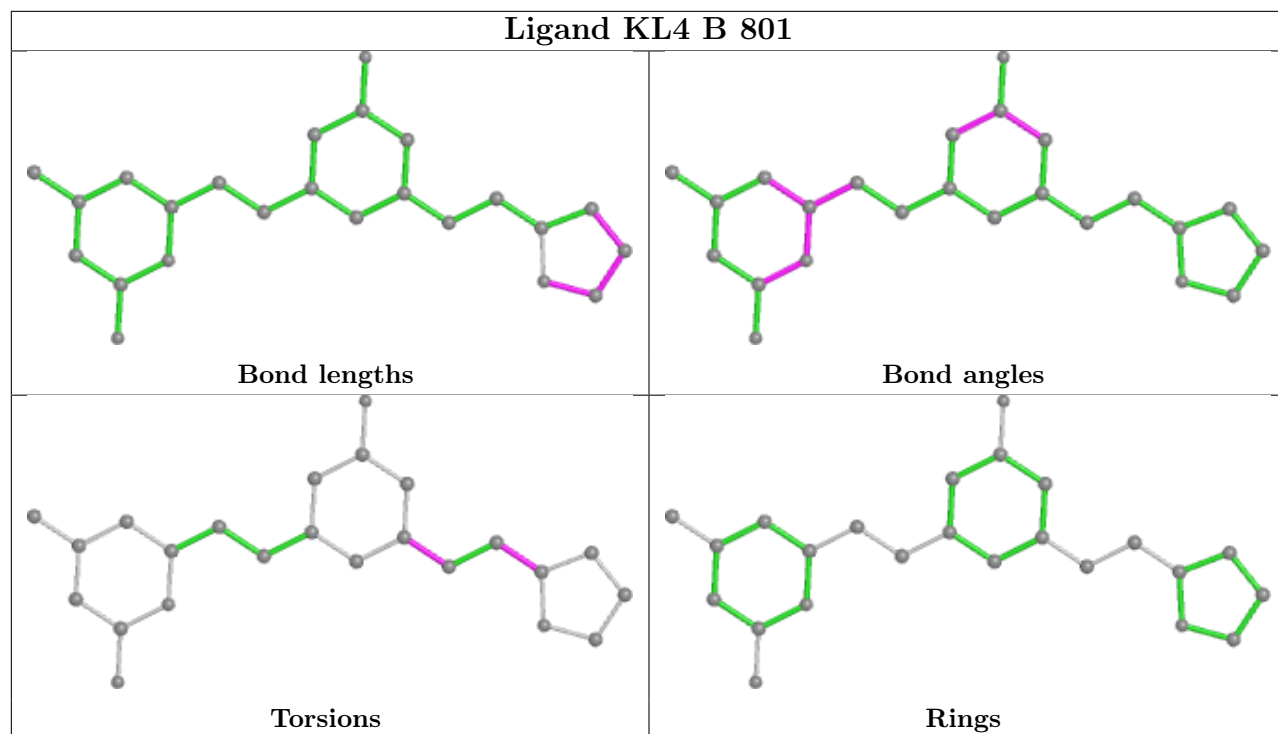




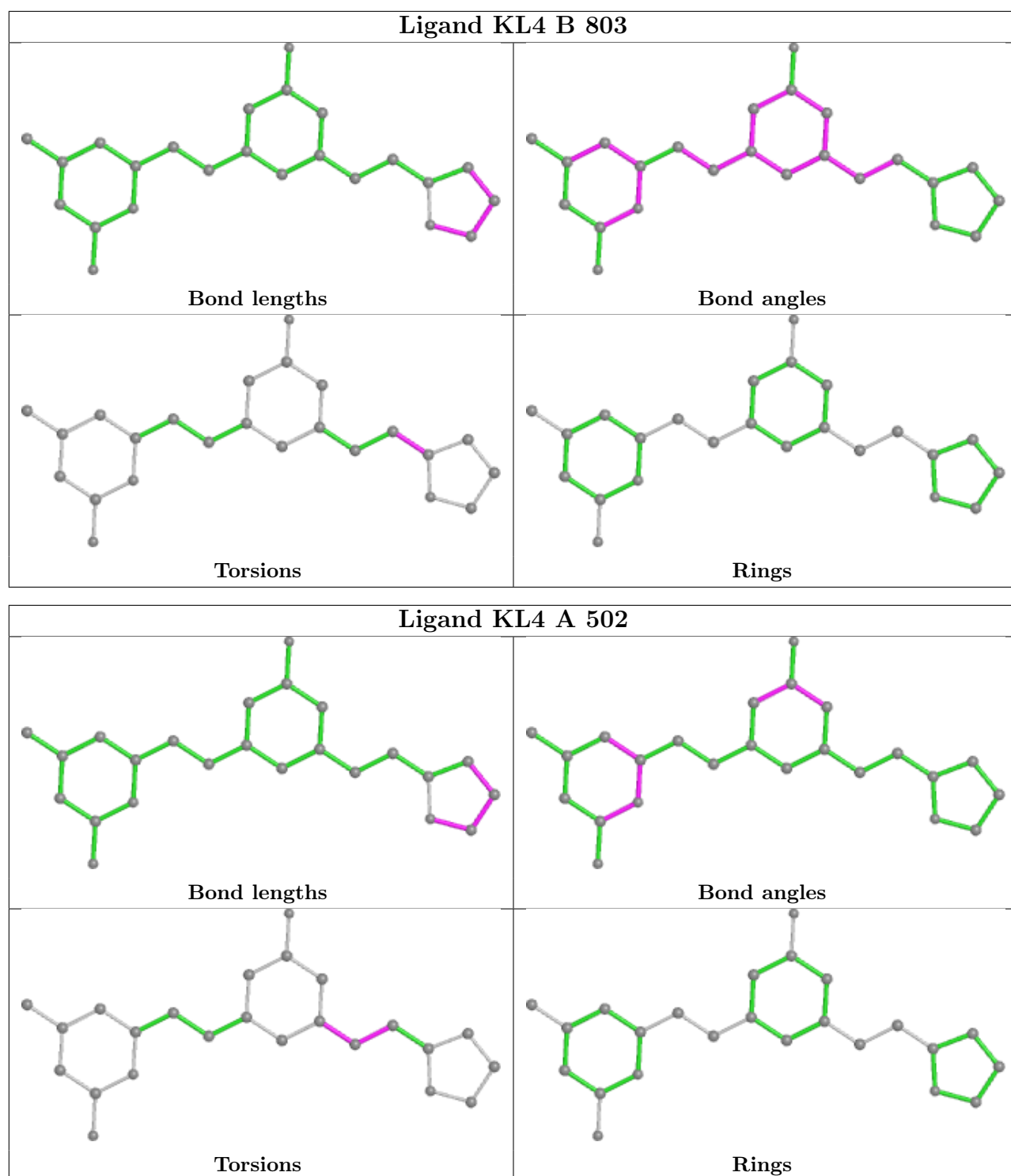












#### 4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues

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.