



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 11:06 AM EDT

PDB ID : 6NH4
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(3-fluoro-5-(2-((2R,4S)-4-fluoropyrrolidin-2-yl)ethyl)phenethyl)-4-methylpyridin-2-amine
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Deposited on : 2018-12-21
Resolution : 2.27 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 2.27 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](#)

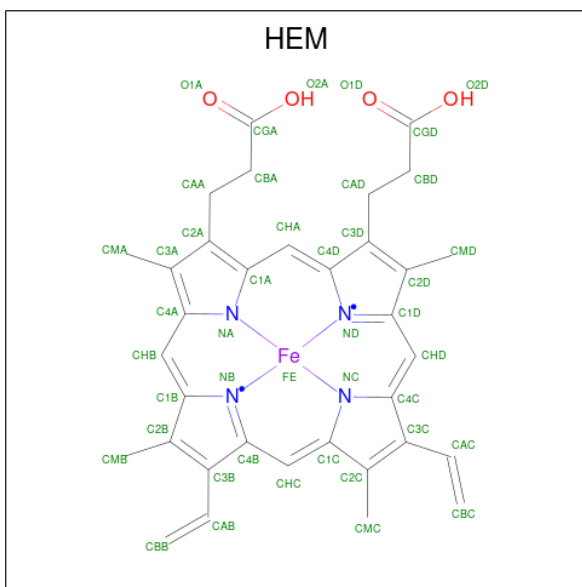
There are 10 unique types of molecules in this entry. The entry contains 14013 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3209	C 2044	N 563	O 586	S 16	0	2	0
1	D	404	Total 3241	C 2063	N 572	O 589	S 17	0	3	0

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



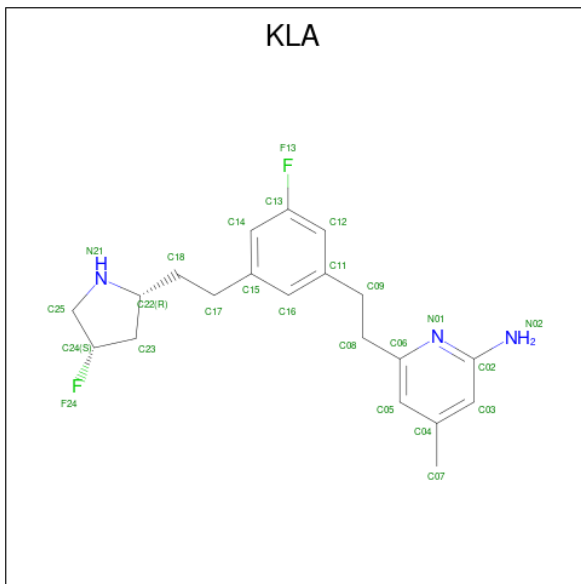
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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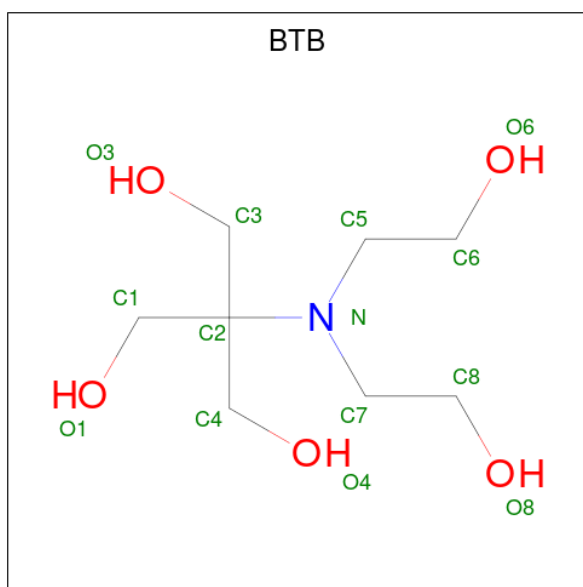
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6-[2-(3-fluoro-5-{2-[(2R,4S)-4-fluoropyrrolidin-2-yl]ethyl}phenyl)ethyl]-4-methylpyridin-2-amine (three-letter code: KLA) (formula: C₂₀H₂₅F₂N₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			25	20	2	3		
3	A	1	Total	C	F	N	0	0
			25	20	2	3		
3	B	1	Total	C	F	N	0	0
			25	20	2	3		
3	C	1	Total	C	F	N	0	0
			25	20	2	3		
3	D	1	Total	C	F	N	0	0
			25	20	2	3		
3	D	1	Total	C	F	N	0	0
			25	20	2	3		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



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	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: C₃H₈O₃).

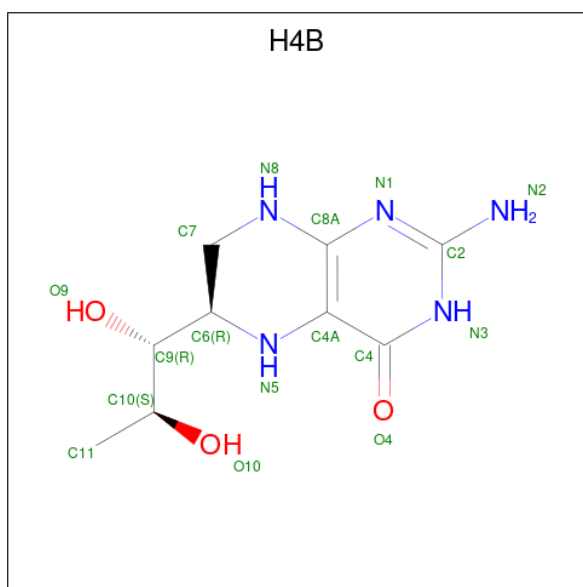


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			6	3 3		
6	C	1	Total	C O	0	0
			6	3 3		

- 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	2	Total	Cl	0	0
			2	2		
7	C	3	Total	Cl	0	0
			3	3		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C₉H₁₅N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			17	9	5	3		
8	C	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 9 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Gd	0	0
			1	1		
9	C	2	Total	Gd	0	0
			2	2		
9	D	1	Total	Gd	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	114	Total	O	0	0
			114	114		
10	B	174	Total	O	0	0
			174	174		
10	C	145	Total	O	0	0
			145	145		
10	D	175	Total	O	0	0
			175	175		

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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.71Å 152.55Å 109.14Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	39.98 – 2.27	Depositor
% Data completeness (in resolution range)	93.3 (39.98-2.27)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.27Å)	Xtrriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, R_{free}	0.192 , 0.251	Depositor
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.412	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtrriage
Total number of atoms	14013	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 39 ligands modelled in this entry, 17 are monoatomic - leaving 22 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
6	GOL	A	507	-	5,5,5	0.39	0	5,5,5	0.40	0
4	BTB	A	504	-	13,13,13	0.40	0	7,16,16	0.68	0
4	BTB	B	508	-	13,13,13	0.68	0	7,16,16	0.62	0
2	HEM	A	501	1	41,50,50	1.53	4 (9%)	45,82,82	1.68	12 (26%)
4	BTB	D	505	-	13,13,13	0.52	0	7,16,16	0.77	0
8	H4B	C	503	-	16,18,18	0.59	0	11,26,26	2.36	5 (45%)
4	BTB	C	505	-	13,13,13	0.38	0	7,16,16	0.39	0
8	H4B	B	501	-	16,18,18	0.64	0	11,26,26	2.37	5 (45%)
3	KLA	A	502	-	26,27,27	0.52	0	31,37,37	1.86	6 (19%)
2	HEM	C	502	1	41,50,50	1.59	5 (12%)	45,82,82	1.76	11 (24%)
2	HEM	B	502	1	41,50,50	1.46	6 (14%)	45,82,82	1.60	10 (22%)
4	BTB	D	504	9	13,13,13	0.58	0	7,16,16	0.85	0
4	BTB	A	503	9	13,13,13	0.46	0	7,16,16	1.06	1 (14%)
4	BTB	B	504	9	13,13,13	0.47	0	7,16,16	0.69	0
6	GOL	C	508	-	5,5,5	0.36	0	5,5,5	0.43	0
2	HEM	D	501	1	41,50,50	1.41	5 (12%)	45,82,82	1.67	11 (24%)
3	KLA	D	502	-	26,27,27	0.54	0	31,37,37	1.46	5 (16%)
3	KLA	C	504	-	26,27,27	0.46	0	31,37,37	1.51	6 (19%)
4	BTB	B	505	-	13,13,13	0.50	0	7,16,16	0.95	1 (14%)
3	KLA	B	503	-	26,27,27	0.70	0	31,37,37	1.57	7 (22%)
3	KLA	A	509	-	26,27,27	0.58	0	31,37,37	1.32	7 (22%)
3	KLA	D	503	-	26,27,27	0.54	0	31,37,37	1.60	6 (19%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	507	-	-	3/4/4/4	-
4	BTB	A	504	-	-	6/21/21/21	-
4	BTB	B	508	-	-	4/21/21/21	-
2	HEM	A	501	1	-	1/12/54/54	-
4	BTB	D	505	-	-	10/21/21/21	-
8	H4B	C	503	-	-	3/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	C	505	-	-	6/21/21/21	-
8	H4B	B	501	-	-	4/8/17/17	0/2/2/2
3	KLA	A	502	-	-	4/10/19/19	0/3/3/3
2	HEM	C	502	1	-	2/12/54/54	-
2	HEM	B	502	1	-	4/12/54/54	-
4	BTB	D	504	9	-	6/21/21/21	-
4	BTB	A	503	9	-	4/21/21/21	-
4	BTB	B	504	9	-	3/21/21/21	-
6	GOL	C	508	-	-	2/4/4/4	-
2	HEM	D	501	1	-	2/12/54/54	-
3	KLA	D	502	-	-	5/10/19/19	0/3/3/3
3	KLA	C	504	-	-	5/10/19/19	0/3/3/3
4	BTB	B	505	-	-	6/21/21/21	-
3	KLA	B	503	-	-	3/10/19/19	0/3/3/3
3	KLA	A	509	-	-	3/10/19/19	0/3/3/3
3	KLA	D	503	-	-	3/10/19/19	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	HEM	FE-NB	4.23	2.17	1.96
2	C	502	HEM	C3C-C2C	-4.03	1.34	1.40
2	A	501	HEM	FE-NB	4.02	2.16	1.96
2	A	501	HEM	C3C-C2C	-3.97	1.34	1.40
2	C	502	HEM	C3C-CAC	3.85	1.55	1.47
2	A	501	HEM	C3C-CAC	3.71	1.55	1.47
2	B	502	HEM	C3C-CAC	3.65	1.55	1.47
2	D	501	HEM	C3C-CAC	3.57	1.55	1.47
2	B	502	HEM	C3C-C2C	-3.28	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.11	1.36	1.40
2	D	501	HEM	CAB-C3B	2.99	1.55	1.47
2	C	502	HEM	CAB-C3B	2.96	1.55	1.47
2	D	501	HEM	FE-NB	2.93	2.11	1.96
2	B	502	HEM	CAB-C3B	2.85	1.55	1.47
2	A	501	HEM	CAB-C3B	2.73	1.54	1.47
2	B	502	HEM	CAA-C2A	2.58	1.55	1.52
2	D	501	HEM	CAA-C2A	2.16	1.55	1.52
2	B	502	HEM	C3B-C2B	-2.16	1.32	1.37
2	C	502	HEM	CMB-C2B	2.13	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	HEM	CMB-C2B	2.01	1.55	1.50

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	KLA	C02-N01-C06	5.62	122.36	118.10
8	B	501	H4B	C8A-C4A-C4	4.72	118.77	114.57
8	C	503	H4B	C8A-C4A-C4	4.70	118.74	114.57
3	C	504	KLA	C02-N01-C06	4.45	121.47	118.10
3	D	503	KLA	C02-N01-C06	4.03	121.16	118.10
3	A	502	KLA	C05-C06-N01	-3.93	118.73	122.90
2	B	502	HEM	CMA-C3A-C4A	-3.74	122.71	128.46
2	C	502	HEM	C4B-CHC-C1C	3.70	127.44	122.56
2	C	502	HEM	CBA-CAA-C2A	-3.68	106.35	112.62
3	B	503	KLA	C14-C13-C12	-3.61	118.95	123.52
8	C	503	H4B	C4-C4A-N5	3.54	122.09	119.12
2	C	502	HEM	C4D-ND-C1D	3.39	108.58	105.07
2	A	501	HEM	C4B-CHC-C1C	3.39	127.03	122.56
8	B	501	H4B	C4-C4A-N5	3.34	121.93	119.12
2	C	502	HEM	C1B-NB-C4B	3.32	108.50	105.07
3	D	502	KLA	C11-C12-C13	3.31	121.82	118.81
2	D	501	HEM	CMC-C2C-C3C	3.28	130.82	124.68
3	D	503	KLA	C09-C08-C06	-3.28	105.65	112.99
3	A	502	KLA	C08-C06-N01	3.27	120.82	115.95
2	C	502	HEM	CBD-CAD-C3D	-3.25	103.59	112.63
2	A	501	HEM	CMA-C3A-C4A	-3.23	123.50	128.46
2	C	502	HEM	CHC-C4B-C3B	3.16	129.41	124.57
3	D	502	KLA	C14-C13-C12	-3.15	119.53	123.52
2	D	501	HEM	C1B-NB-C4B	3.10	108.28	105.07
2	D	501	HEM	C4D-ND-C1D	3.09	108.27	105.07
2	C	502	HEM	C3D-C4D-ND	-3.08	106.73	110.17
2	D	501	HEM	CBD-CAD-C3D	-3.05	104.14	112.63
3	A	502	KLA	C14-C13-C12	-3.02	119.70	123.52
2	A	501	HEM	C1B-NB-C4B	3.00	108.17	105.07
3	B	503	KLA	C08-C06-N01	2.99	120.41	115.95
3	C	504	KLA	C14-C13-C12	-2.99	119.75	123.52
2	B	502	HEM	CMA-C3A-C2A	2.98	130.56	124.94
2	D	501	HEM	C4B-CHC-C1C	2.94	126.44	122.56
2	A	501	HEM	C3B-C2B-C1B	2.88	108.62	106.49
3	D	503	KLA	C04-C05-C06	-2.81	118.48	120.32
3	D	503	KLA	C14-C13-C12	-2.81	119.97	123.52
2	A	501	HEM	CBD-CAD-C3D	-2.79	104.88	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C3B-C2B-C1B	2.79	108.56	106.49
8	B	501	H4B	C2-N3-C4	2.79	120.36	115.93
2	B	502	HEM	CAB-C3B-C2B	-2.70	119.72	128.60
2	A	501	HEM	C4D-ND-C1D	2.64	107.80	105.07
3	B	503	KLA	C11-C12-C13	2.61	121.19	118.81
3	A	509	KLA	C14-C13-C12	-2.60	120.23	123.52
8	C	503	H4B	C2-N3-C4	2.60	120.06	115.93
8	C	503	H4B	C2-N1-C8A	2.57	120.31	114.54
3	B	503	KLA	C02-N01-C06	2.57	120.05	118.10
2	D	501	HEM	C3D-C4D-ND	-2.54	107.34	110.17
2	A	501	HEM	CAA-CBA-CGA	-2.52	106.68	113.76
2	B	502	HEM	CHA-C4D-ND	2.52	127.49	124.38
2	B	502	HEM	CMC-C2C-C3C	2.51	129.38	124.68
2	B	502	HEM	C4D-ND-C1D	2.51	107.67	105.07
3	D	503	KLA	C18-C22-C23	-2.49	109.26	113.50
3	C	504	KLA	C05-C06-N01	-2.49	120.26	122.90
2	D	501	HEM	CMA-C3A-C4A	-2.49	124.64	128.46
3	A	502	KLA	C11-C12-C13	2.46	121.04	118.81
2	A	501	HEM	C3D-C4D-ND	-2.41	107.49	110.17
2	A	501	HEM	CHA-C4D-ND	2.41	127.35	124.38
3	A	509	KLA	C02-N01-C06	2.41	119.92	118.10
3	B	503	KLA	F13-C13-C12	2.40	121.67	118.25
2	B	502	HEM	CBD-CAD-C3D	-2.39	105.98	112.63
8	C	503	H4B	N1-C2-N3	-2.39	121.67	125.42
3	D	502	KLA	C02-N01-C06	2.39	119.91	118.10
8	B	501	H4B	C2-N1-C8A	2.39	119.89	114.54
8	B	501	H4B	N1-C2-N3	-2.36	121.71	125.42
2	C	502	HEM	C3B-C2B-C1B	2.34	108.22	106.49
2	B	502	HEM	C3B-C2B-C1B	2.33	108.21	106.49
3	D	503	KLA	C08-C06-N01	2.32	119.40	115.95
2	C	502	HEM	CHD-C1D-ND	2.31	126.94	124.43
2	D	501	HEM	CAB-C3B-C2B	-2.30	121.03	128.60
3	A	509	KLA	C08-C06-N01	2.29	119.37	115.95
3	B	503	KLA	C05-C06-N01	-2.29	120.47	122.90
3	A	509	KLA	C18-C22-C23	-2.25	109.67	113.50
3	D	502	KLA	C08-C09-C11	-2.25	105.38	113.28
3	C	504	KLA	C08-C06-N01	2.24	119.29	115.95
2	B	502	HEM	C4B-CHC-C1C	2.23	125.51	122.56
2	C	502	HEM	CHA-C4D-ND	2.21	127.11	124.38
2	A	501	HEM	CHC-C4B-C3B	2.14	127.84	124.57
2	D	501	HEM	CHA-C4D-ND	2.14	127.02	124.38
3	A	509	KLA	C09-C08-C06	-2.10	108.29	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	HEM	CAA-CBA-CGA	-2.10	107.88	113.76
2	A	501	HEM	CBA-CAA-C2A	-2.09	109.06	112.62
2	A	501	HEM	CMA-C3A-C2A	2.08	128.86	124.94
2	C	502	HEM	CMA-C3A-C4A	-2.08	125.27	128.46
3	A	509	KLA	F13-C13-C12	2.08	121.22	118.25
3	A	502	KLA	N02-C02-N01	2.07	119.76	116.49
4	A	503	BTB	O3-C3-C2	-2.06	105.80	111.44
3	D	502	KLA	C16-C15-C14	2.06	121.81	118.98
3	C	504	KLA	C11-C12-C13	2.05	120.67	118.81
2	D	501	HEM	C2B-C1B-NB	-2.03	107.43	109.84
3	C	504	KLA	F13-C13-C12	2.03	121.16	118.25
3	B	503	KLA	C18-C22-C23	-2.03	110.04	113.50
3	A	509	KLA	N02-C02-N01	2.01	119.67	116.49
4	B	505	BTB	O4-C4-C2	-2.01	105.95	111.44

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	HEM	C1A-C2A-CAA-CBA
2	B	502	HEM	C3A-C2A-CAA-CBA
3	A	502	KLA	C17-C18-C22-C23
3	A	502	KLA	C17-C18-C22-N21
3	A	509	KLA	C15-C17-C18-C22
3	A	509	KLA	C17-C18-C22-C23
3	A	509	KLA	C17-C18-C22-N21
3	B	503	KLA	C15-C17-C18-C22
3	C	504	KLA	C15-C17-C18-C22
3	D	502	KLA	C15-C17-C18-C22
3	D	503	KLA	C15-C17-C18-C22
4	A	503	BTB	O1-C1-C2-C3
4	A	503	BTB	O1-C1-C2-C4
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	B	504	BTB	O1-C1-C2-C3
4	B	504	BTB	O1-C1-C2-C4
4	B	504	BTB	O1-C1-C2-N
4	B	505	BTB	C1-C2-C4-O4
4	B	505	BTB	C3-C2-C4-O4
4	B	508	BTB	C1-C2-C3-O3
4	B	508	BTB	C4-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	508	BTB	N-C2-C3-O3
4	B	508	BTB	C8-C7-N-C5
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	D	504	BTB	O1-C1-C2-C3
4	D	504	BTB	O1-C1-C2-N
4	D	505	BTB	O1-C1-C2-C4
4	D	505	BTB	C1-C2-N-C7
4	D	505	BTB	C8-C7-N-C5
6	A	507	GOL	O1-C1-C2-C3
6	C	508	GOL	O1-C1-C2-O2
6	C	508	GOL	O1-C1-C2-C3
8	B	501	H4B	N5-C6-C9-O9
8	B	501	H4B	C7-C6-C9-O9
8	B	501	H4B	C7-C6-C9-C10
8	C	503	H4B	C7-C6-C9-O9
8	C	503	H4B	C7-C6-C9-C10
4	A	504	BTB	N-C7-C8-O8
2	A	501	HEM	C2A-CAA-CBA-CGA
2	B	502	HEM	C2A-CAA-CBA-CGA
2	C	502	HEM	C2A-CAA-CBA-CGA
2	D	501	HEM	C2A-CAA-CBA-CGA
4	D	504	BTB	N-C5-C6-O6
6	A	507	GOL	O1-C1-C2-O2
2	B	502	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
4	D	505	BTB	N-C7-C8-O8
2	C	502	HEM	C4B-C3B-CAB-CBB
3	D	503	KLA	C17-C18-C22-N21
8	C	503	H4B	N5-C6-C9-O9
3	C	504	KLA	C17-C18-C22-C23
3	D	502	KLA	C17-C18-C22-C23
3	D	503	KLA	C17-C18-C22-C23
4	D	504	BTB	O1-C1-C2-C4
4	D	504	BTB	C1-C2-C3-O3
4	D	504	BTB	C4-C2-C3-O3
4	D	505	BTB	O1-C1-C2-C3
4	A	503	BTB	O1-C1-C2-N
4	B	505	BTB	N-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
4	C	505	BTB	N-C2-C4-O4
4	D	505	BTB	O1-C1-C2-N
4	D	505	BTB	C3-C2-N-C5
4	D	505	BTB	C3-C2-N-C7
4	D	505	BTB	C4-C2-N-C5
4	D	505	BTB	C4-C2-N-C7
4	B	505	BTB	N-C5-C6-O6
8	B	501	H4B	N5-C6-C9-C10
3	A	502	KLA	C14-C15-C17-C18
3	A	502	KLA	C16-C15-C17-C18
3	B	503	KLA	C14-C15-C17-C18
3	B	503	KLA	C16-C15-C17-C18
3	D	502	KLA	C14-C15-C17-C18
3	D	502	KLA	C16-C15-C17-C18
3	C	504	KLA	C14-C15-C17-C18
3	C	504	KLA	C16-C15-C17-C18
6	A	507	GOL	O2-C2-C3-O3
3	C	504	KLA	C17-C18-C22-N21
3	D	502	KLA	C17-C18-C22-N21
4	A	503	BTB	N-C7-C8-O8
4	A	504	BTB	C1-C2-C4-O4
4	A	504	BTB	C3-C2-C4-O4
4	B	505	BTB	C1-C2-C3-O3
4	B	505	BTB	C4-C2-C3-O3

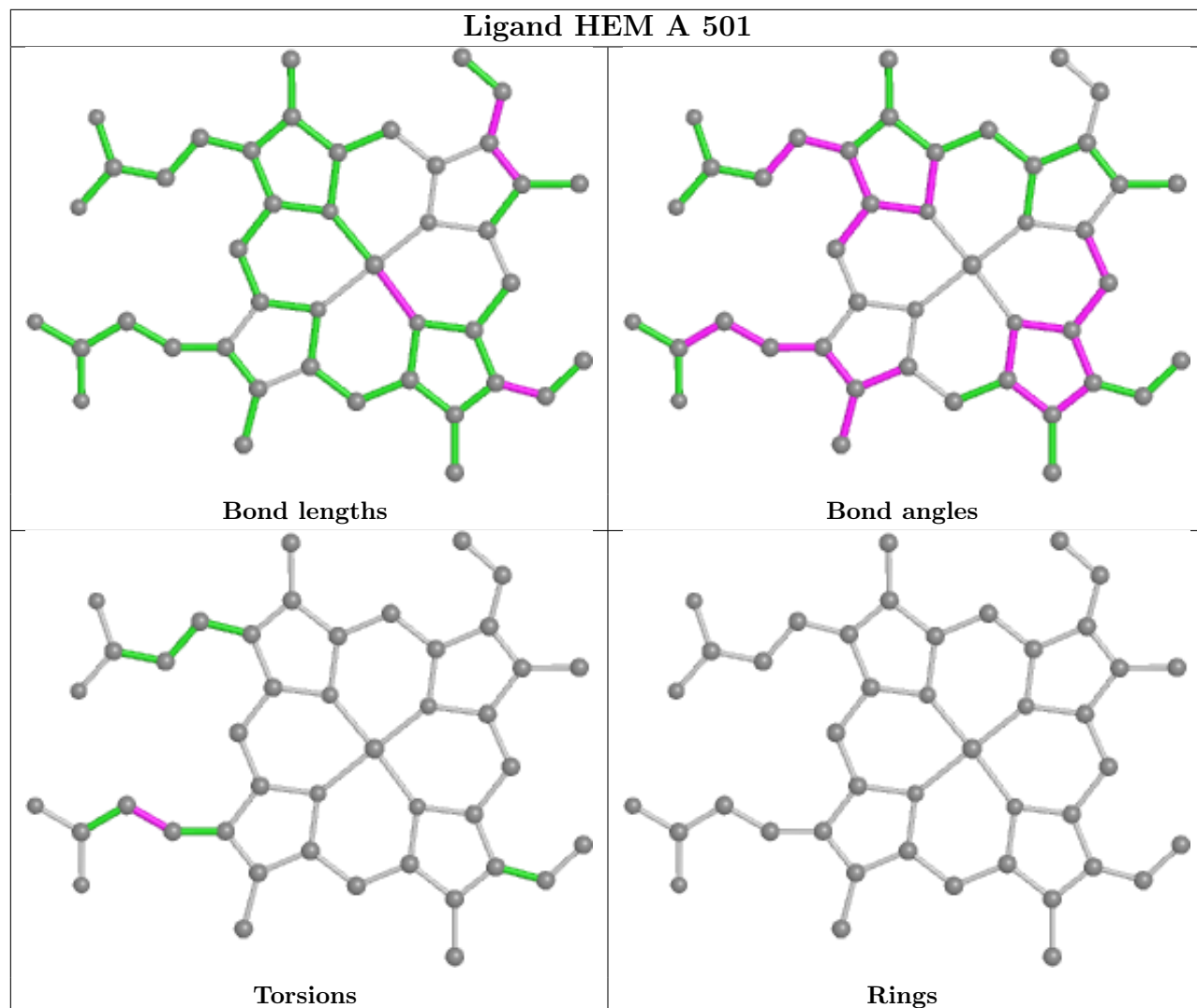
There are no ring outliers.

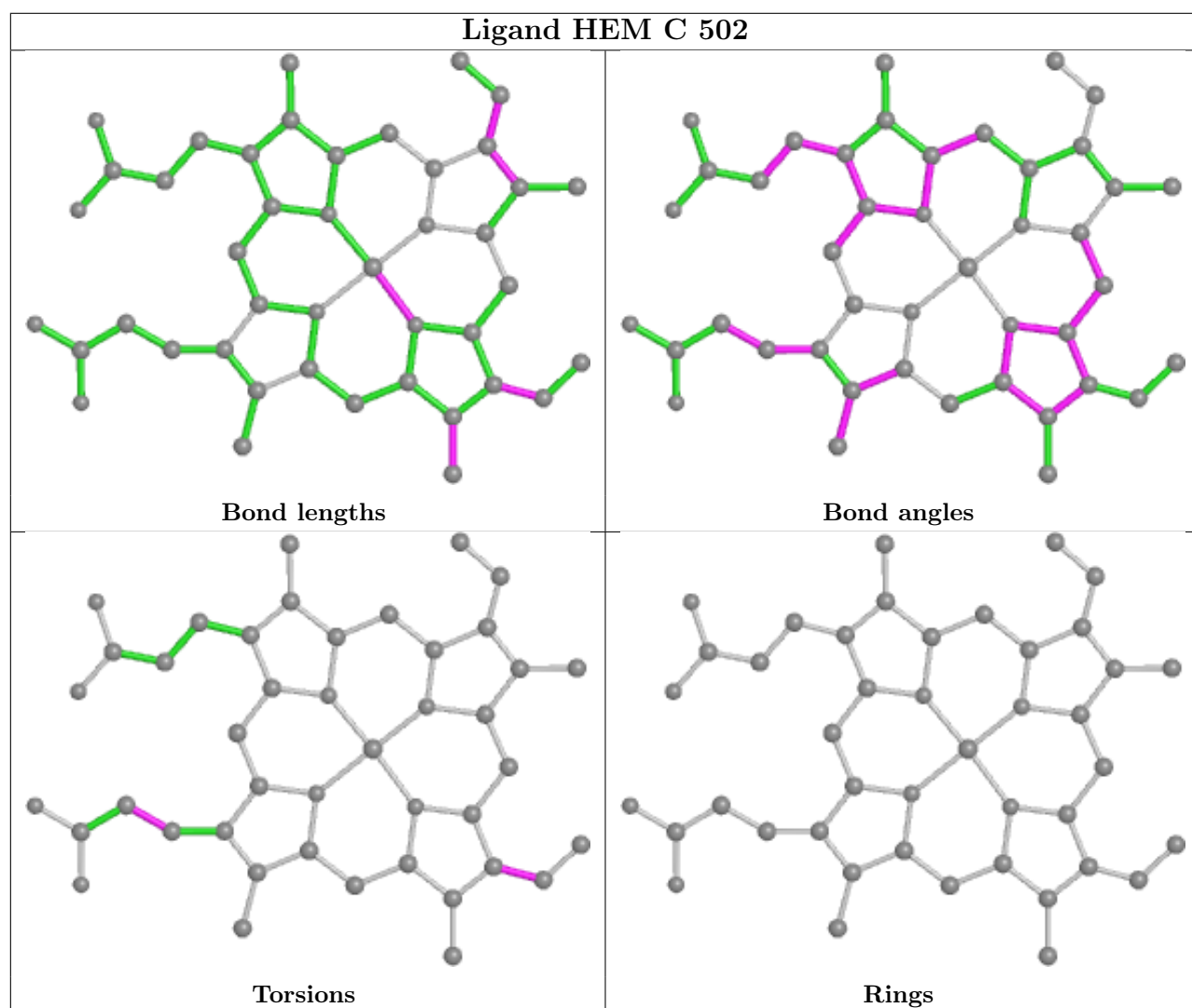
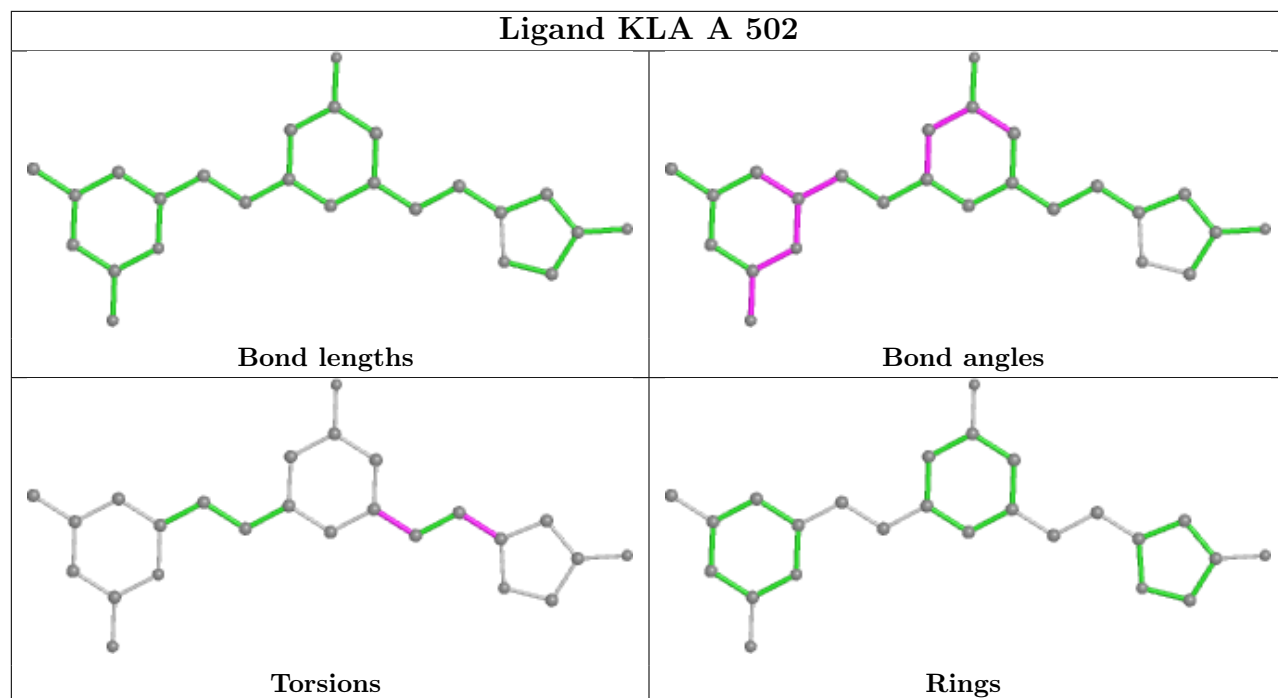
1 monomer is involved in 1 short contact:

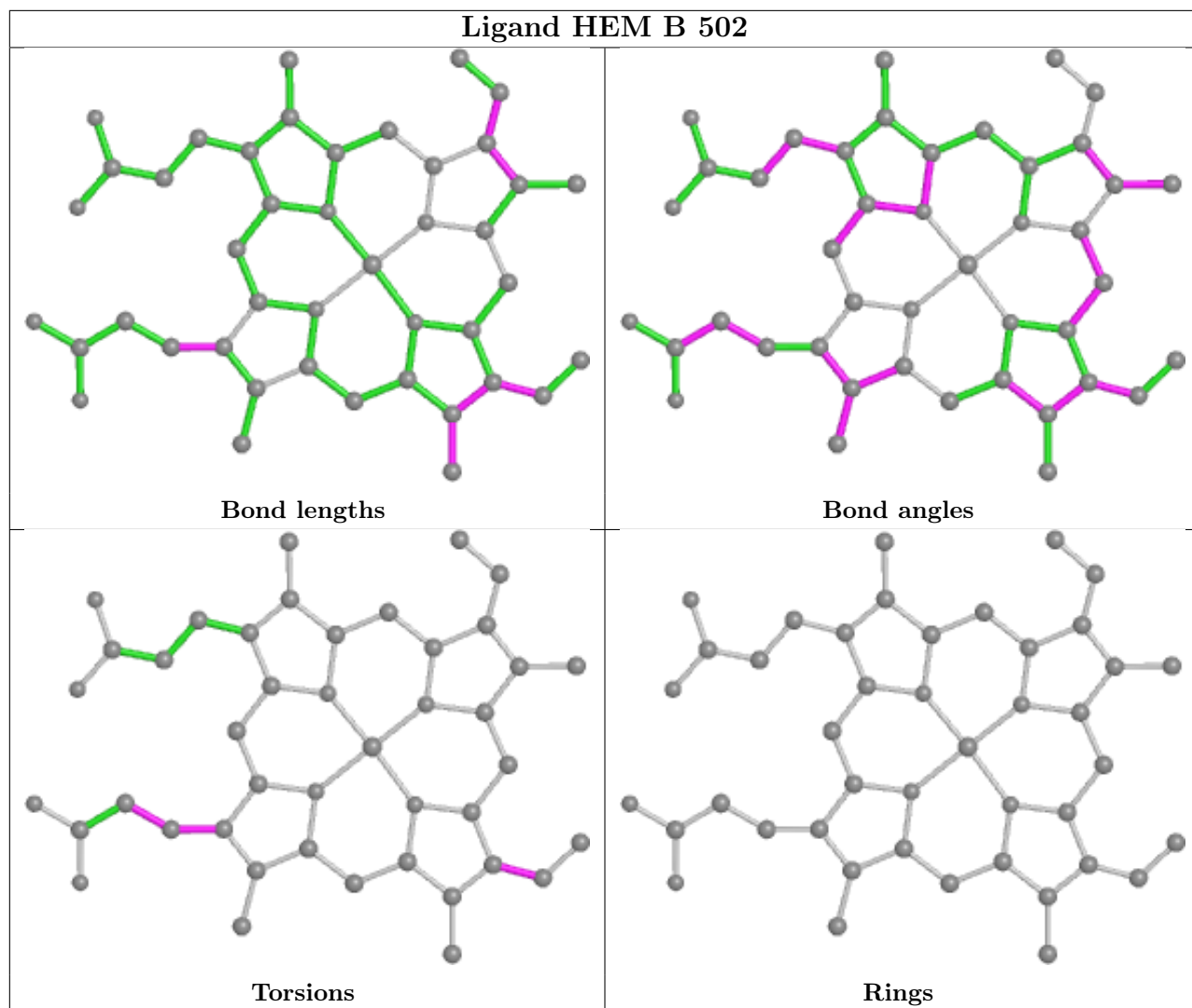
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	505	BTB	0	1

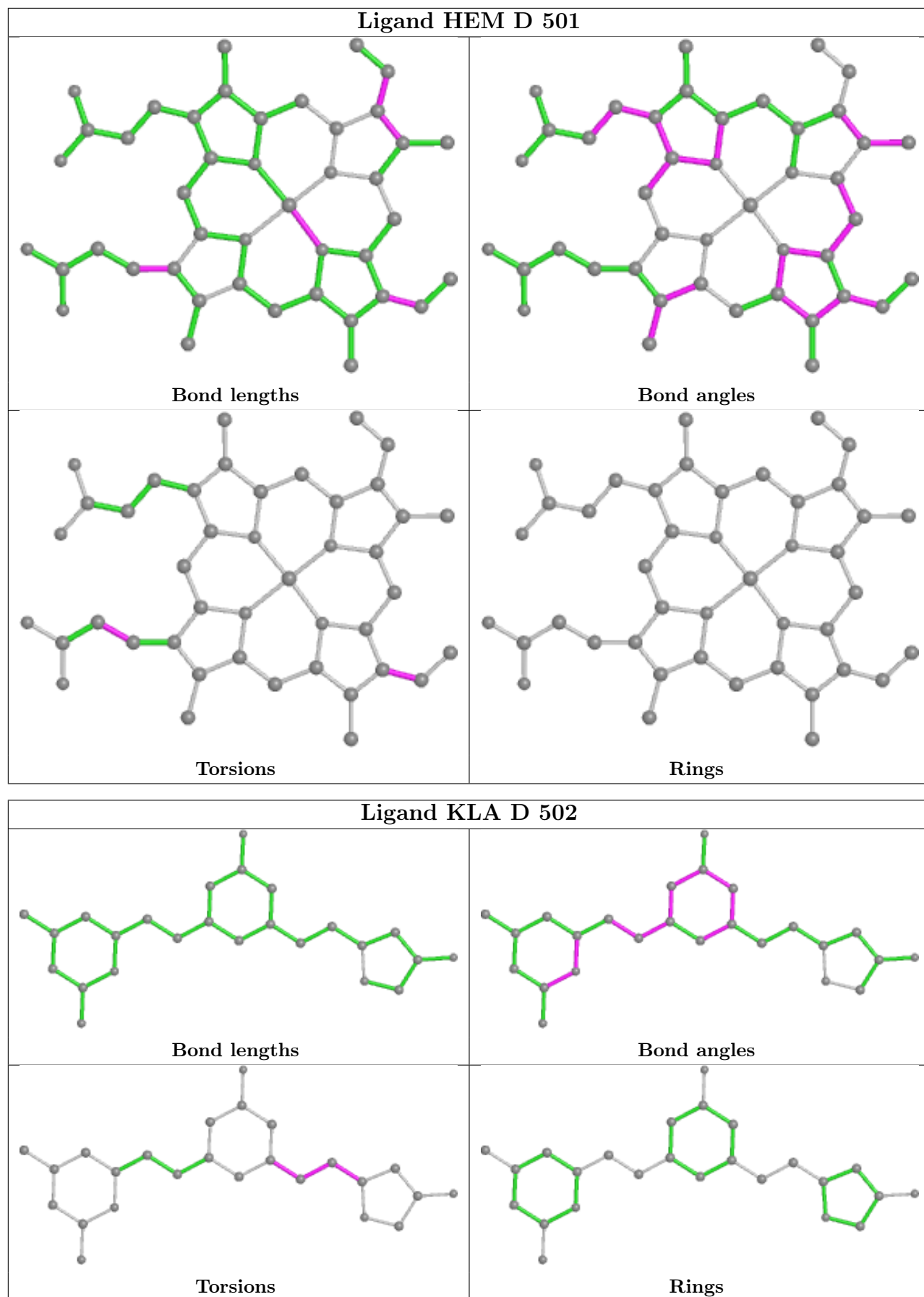
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

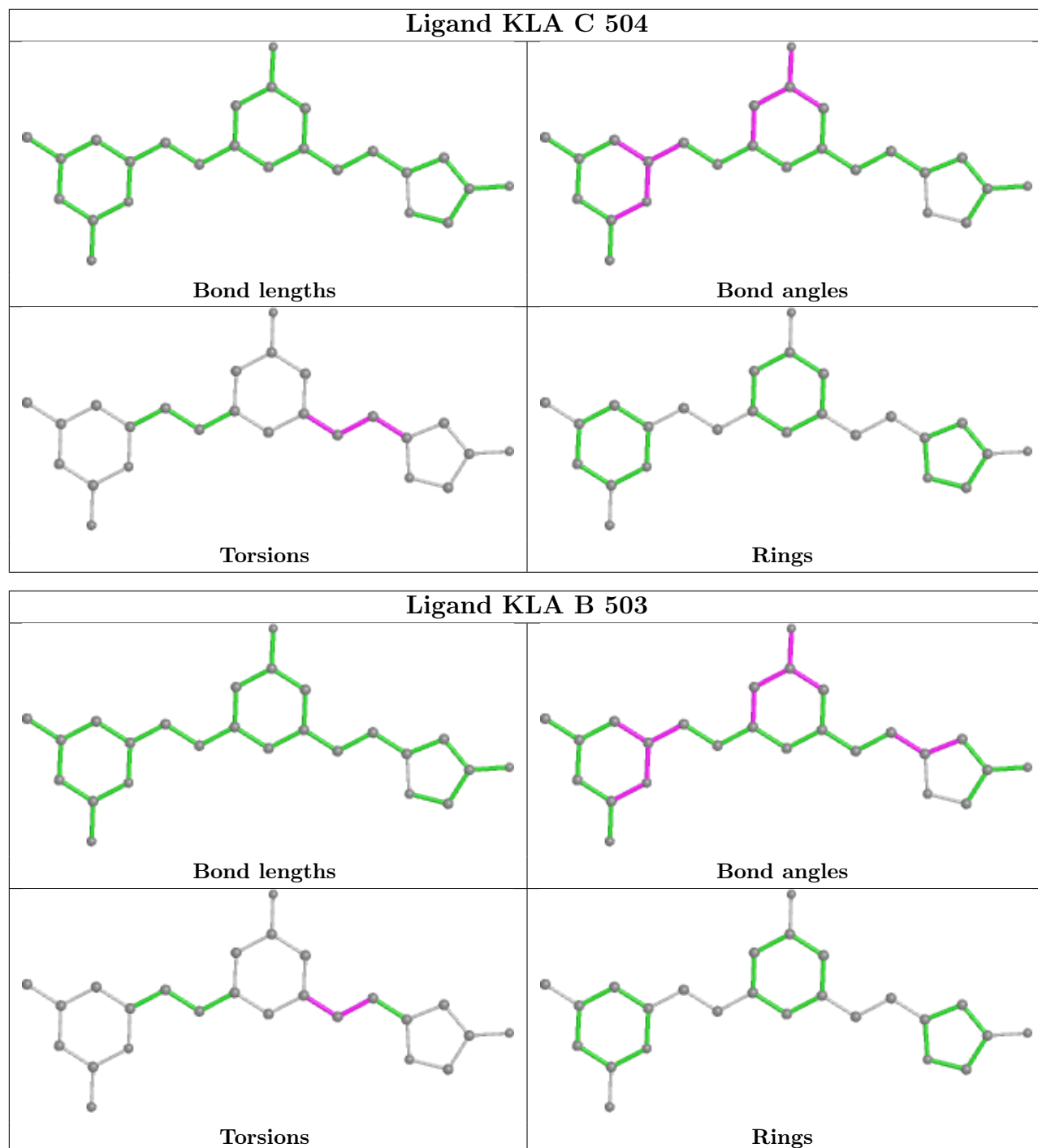
equivalents in the CSD to analyse the geometry.

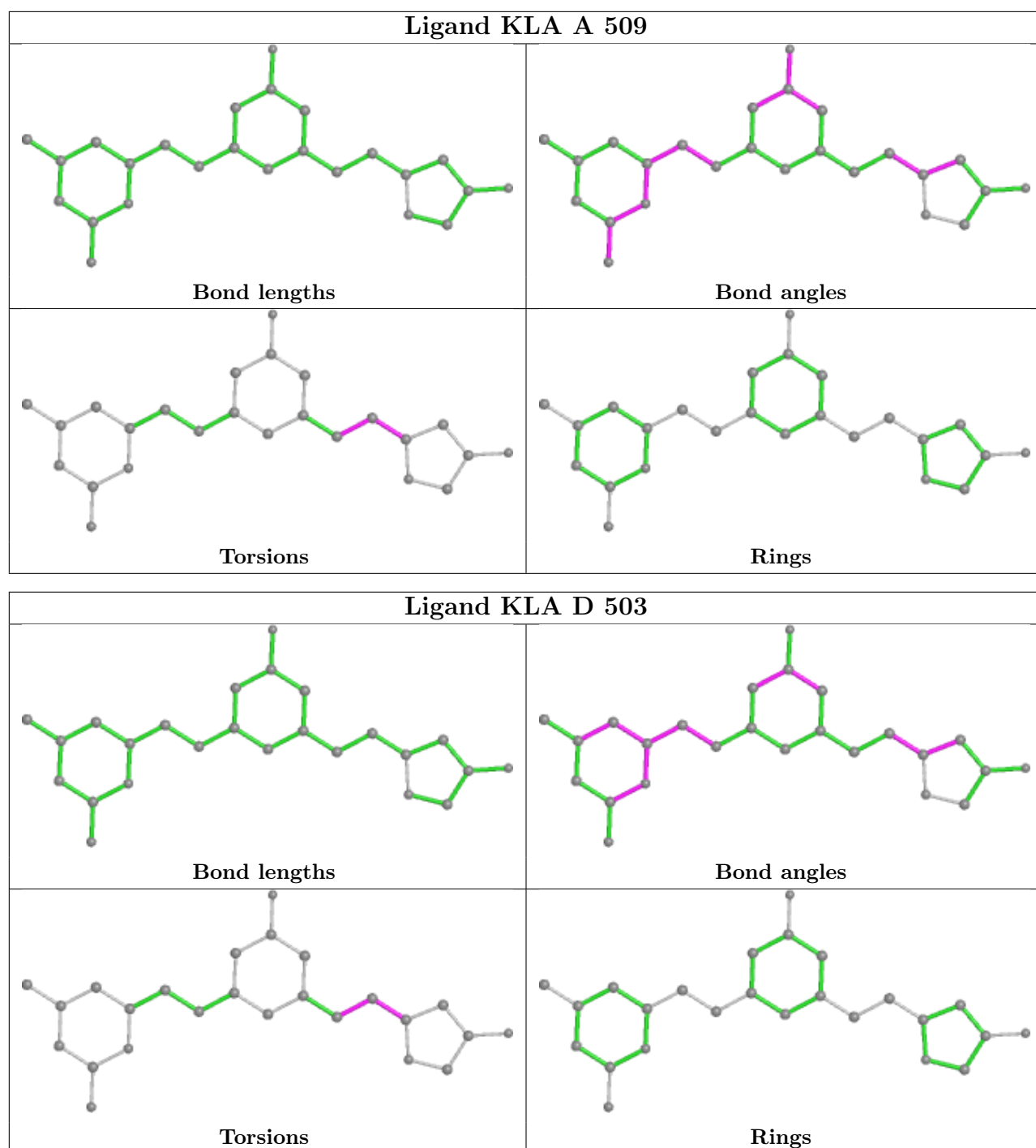












4.7 Other polymers [\(i\)](#)

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.