



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 11:04 AM EDT

PDB ID : 6MN4
Title : Crystal structure of aminoglycoside acetyltransferase AAC(3)-IVa, H154A mutant, in complex with apramycin
Authors : Stogios, P.J.; Evdokimova, E.; Michalska, K.; Di Leo, R.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2018-10-01
Resolution : 2.80 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 2.80 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 8 unique types of molecules in this entry. The entry contains 12349 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 Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	1957	1243	347	359	8	0	0	0
1	B	258	1961	1246	348	359	8	0	0	0
1	C	258	1961	1246	348	359	8	0	0	0
1	D	258	1961	1246	348	359	8	0	0	0
1	E	258	1954	1240	347	359	8	0	0	0
1	F	242	1833	1164	325	336	8	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

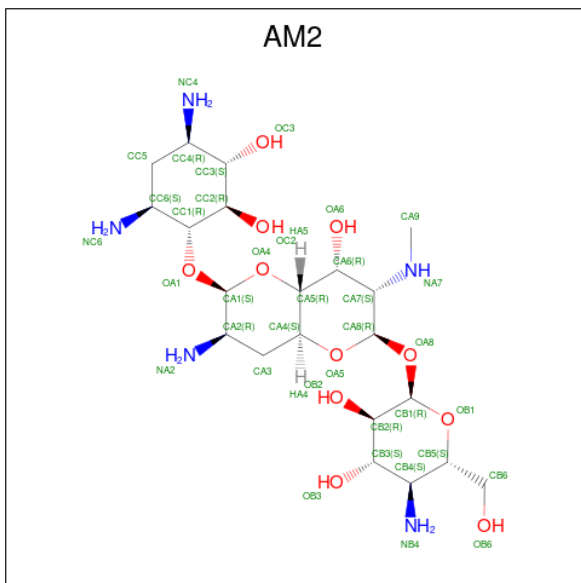
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP Q306W4
A	0	GLY	-	expression tag	UNP Q306W4
A	154	ALA	HIS	engineered mutation	UNP Q306W4
B	-1	GLN	-	expression tag	UNP Q306W4
B	0	GLY	-	expression tag	UNP Q306W4
B	154	ALA	HIS	engineered mutation	UNP Q306W4
C	-1	GLN	-	expression tag	UNP Q306W4
C	0	GLY	-	expression tag	UNP Q306W4
C	154	ALA	HIS	engineered mutation	UNP Q306W4
D	-1	GLN	-	expression tag	UNP Q306W4
D	0	GLY	-	expression tag	UNP Q306W4
D	154	ALA	HIS	engineered mutation	UNP Q306W4
E	-1	GLN	-	expression tag	UNP Q306W4
E	0	GLY	-	expression tag	UNP Q306W4
E	154	ALA	HIS	engineered mutation	UNP Q306W4
F	-1	GLN	-	expression tag	UNP Q306W4
F	0	GLY	-	expression tag	UNP Q306W4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	154	ALA	HIS	engineered mutation	UNP Q306W4

- Molecule 2 is APRAMYCIN (three-letter code: AM2) (formula: C₂₁H₄₁N₅O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			37	21	5	11		
2	B	1	Total	C	N	O	0	0
			37	21	5	11		
2	C	1	Total	C	N	O	0	0
			37	21	5	11		
2	D	1	Total	C	N	O	0	0
			37	21	5	11		
2	E	1	Total	C	N	O	0	0
			37	21	5	11		
2	F	1	Total	C	N	O	0	0
			37	21	5	11		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



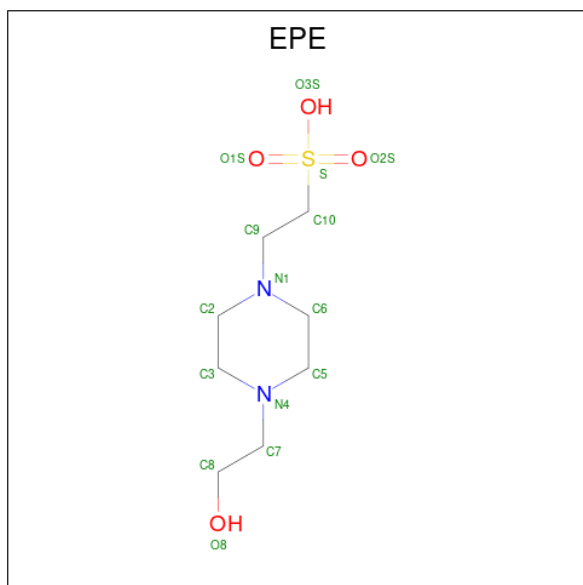
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	77	Total O 77 77	0	0
8	B	100	Total O 100 100	0	0
8	C	49	Total O 50 50	0	1
8	D	49	Total O 49 49	0	0
8	E	36	Total O 36 36	0	0
8	F	28	Total O 28 28	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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.55Å 130.51Å 264.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.33 – 2.80	Depositor
% Data completeness (in resolution range)	94.7 (29.33-2.80)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.07 (at 2.72Å)	Xtrriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, R_{free}	0.247 , 0.304	Depositor
Wilson B-factor (Å ²)	51.5	Xtrriage
Anisotropy	0.384	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12349	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 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	AM2	F	301	-	40,40,40	1.68	7 (17%)	53,60,60	1.40	6 (11%)
4	EDO	A	303	-	3,3,3	0.49	0	2,2,2	0.25	0
7	GOL	D	304	-	5,5,5	0.92	0	5,5,5	0.99	0
2	AM2	A	301	-	40,40,40	1.67	8 (20%)	53,60,60	1.42	7 (13%)
6	EPE	E	305	-	15,15,15	0.74	1 (6%)	18,20,20	1.81	5 (27%)
7	GOL	E	304	-	5,5,5	0.92	0	5,5,5	1.00	0
4	EDO	E	302	-	3,3,3	0.46	0	2,2,2	0.37	0
2	AM2	C	301	-	40,40,40	1.64	7 (17%)	53,60,60	1.10	2 (3%)
5	PO4	F	302	-	4,4,4	0.92	0	6,6,6	0.43	0
5	PO4	A	307	-	4,4,4	0.89	0	6,6,6	0.48	0
2	AM2	D	301	-	40,40,40	1.70	6 (15%)	53,60,60	1.27	5 (9%)
5	PO4	B	304	-	4,4,4	0.91	0	6,6,6	0.48	0
6	EPE	A	308	-	15,15,15	0.70	1 (6%)	18,20,20	1.95	6 (33%)
4	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.36	0
6	EPE	F	303	-	15,15,15	3.20	1 (6%)	18,20,20	2.27	7 (38%)
2	AM2	B	301	-	40,40,40	1.74	6 (15%)	53,60,60	1.45	10 (18%)
5	PO4	C	303	-	4,4,4	0.87	0	6,6,6	0.53	0
6	EPE	B	305	-	15,15,15	0.73	1 (6%)	18,20,20	1.94	5 (27%)
4	EDO	B	303	-	3,3,3	0.48	0	2,2,2	0.28	0
5	PO4	D	303	-	4,4,4	0.92	0	6,6,6	0.46	0
2	AM2	E	301	-	40,40,40	1.69	8 (20%)	53,60,60	1.35	5 (9%)
4	EDO	A	306	-	3,3,3	0.47	0	2,2,2	0.33	0
6	EPE	C	304	-	15,15,15	0.78	1 (6%)	18,20,20	1.68	6 (33%)
5	PO4	E	303	-	4,4,4	0.90	0	6,6,6	0.44	0
4	EDO	A	305	-	3,3,3	0.46	0	2,2,2	0.36	0
6	EPE	D	305	-	15,15,15	0.69	1 (6%)	18,20,20	1.81	4 (22%)

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	AM2	F	301	-	-	10/12/84/84	0/4/4/4
4	EDO	A	303	-	-	0/1/1/1	-
7	GOL	D	304	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AM2	A	301	-	-	10/12/84/84	0/4/4/4
6	EPE	E	305	-	-	5/9/19/19	0/1/1/1
7	GOL	E	304	-	-	0/4/4/4	-
4	EDO	E	302	-	-	0/1/1/1	-
2	AM2	C	301	-	-	9/12/84/84	1/4/4/4
2	AM2	D	301	-	-	8/12/84/84	0/4/4/4
6	EPE	A	308	-	-	7/9/19/19	0/1/1/1
4	EDO	A	304	-	-	1/1/1/1	-
6	EPE	F	303	-	-	1/9/19/19	0/1/1/1
2	AM2	B	301	-	-	8/12/84/84	0/4/4/4
6	EPE	B	305	-	-	4/9/19/19	0/1/1/1
4	EDO	B	303	-	-	0/1/1/1	-
2	AM2	E	301	-	-	10/12/84/84	0/4/4/4
4	EDO	A	306	-	-	0/1/1/1	-
6	EPE	C	304	-	-	3/9/19/19	0/1/1/1
4	EDO	A	305	-	-	0/1/1/1	-
6	EPE	D	305	-	-	5/9/19/19	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	303	EPE	C10-S	-12.21	1.60	1.77
2	B	301	AM2	OA4-CA1	4.65	1.53	1.41
2	D	301	AM2	OA4-CA1	4.58	1.53	1.41
2	C	301	AM2	OA4-CA1	4.42	1.53	1.41
2	F	301	AM2	OA4-CA1	4.40	1.53	1.41
2	E	301	AM2	OA4-CA1	4.40	1.53	1.41
2	A	301	AM2	OA4-CA1	4.38	1.53	1.41
2	D	301	AM2	OA4-CA5	3.89	1.50	1.44
2	D	301	AM2	OA5-CA8	3.75	1.51	1.41
2	E	301	AM2	OA4-CA5	3.74	1.49	1.44
2	F	301	AM2	OA5-CA8	3.74	1.51	1.41
2	E	301	AM2	OA5-CA8	3.71	1.51	1.41
2	B	301	AM2	OA5-CA8	3.67	1.51	1.41
2	F	301	AM2	OA4-CA5	3.67	1.49	1.44
2	A	301	AM2	OA4-CA5	3.66	1.49	1.44
2	B	301	AM2	OA4-CA5	3.62	1.49	1.44
2	C	301	AM2	OA5-CA8	3.59	1.51	1.41
2	A	301	AM2	OA5-CA8	3.54	1.50	1.41
2	F	301	AM2	OA5-CA4	3.35	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	AM2	OA5-CA4	3.33	1.52	1.44
2	C	301	AM2	OA4-CA5	3.30	1.49	1.44
2	A	301	AM2	OA5-CA4	3.30	1.52	1.44
2	D	301	AM2	OB1-CB1	3.22	1.50	1.41
2	D	301	AM2	OA5-CA4	3.21	1.52	1.44
2	B	301	AM2	OA5-CA4	3.20	1.52	1.44
2	B	301	AM2	OB1-CB1	3.19	1.50	1.41
2	C	301	AM2	OB1-CB1	3.15	1.49	1.41
2	F	301	AM2	OB1-CB1	3.12	1.49	1.41
2	E	301	AM2	OB1-CB1	3.11	1.49	1.41
2	D	301	AM2	CB3-CB4	-3.10	1.49	1.53
2	A	301	AM2	OB1-CB1	3.07	1.49	1.41
2	C	301	AM2	OA5-CA4	2.96	1.51	1.44
2	E	301	AM2	CB3-CB4	-2.89	1.49	1.53
2	A	301	AM2	CB3-CB4	-2.84	1.50	1.53
2	F	301	AM2	CB3-CB4	-2.82	1.50	1.53
2	C	301	AM2	CB3-CB4	-2.82	1.50	1.53
2	B	301	AM2	CB3-CB4	-2.78	1.50	1.53
6	C	304	EPE	C10-S	2.44	1.81	1.77
6	E	305	EPE	C10-S	2.36	1.80	1.77
6	B	305	EPE	C10-S	2.29	1.80	1.77
6	A	308	EPE	C10-S	2.24	1.80	1.77
2	A	301	AM2	OA8-CA8	-2.18	1.35	1.41
6	D	305	EPE	C10-S	2.16	1.80	1.77
2	A	301	AM2	OA1-CA1	-2.12	1.35	1.41
2	E	301	AM2	OA1-CA1	-2.09	1.35	1.41
2	F	301	AM2	OA8-CA8	-2.06	1.36	1.41
2	E	301	AM2	OA8-CA8	-2.03	1.36	1.41
2	C	301	AM2	OA8-CA8	-2.03	1.36	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	303	EPE	O3S-S-C10	5.45	114.59	105.77
6	A	308	EPE	C5-N4-C3	5.36	120.90	108.83
2	F	301	AM2	CC6-CC5-CC4	4.51	120.44	111.18
2	A	301	AM2	CC6-CC5-CC4	4.49	120.39	111.18
6	D	305	EPE	C5-N4-C3	4.44	118.81	108.83
6	E	305	EPE	C5-N4-C3	4.43	118.80	108.83
6	B	305	EPE	C5-N4-C3	4.30	118.50	108.83
2	E	301	AM2	CC6-CC5-CC4	4.26	119.94	111.18
2	A	301	AM2	CC5-CC4-CC3	4.07	116.18	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	305	EPE	C7-N4-C5	3.85	121.08	111.23
2	F	301	AM2	CC5-CC4-CC3	3.78	115.74	110.04
6	F	303	EPE	O1S-S-C10	3.71	111.38	106.92
2	D	301	AM2	CC6-CC5-CC4	3.58	118.53	111.18
2	B	301	AM2	OA5-CA4-CA5	3.53	117.19	109.75
6	C	304	EPE	O2S-S-C10	3.48	111.11	106.92
6	D	305	EPE	C7-N4-C5	3.47	120.11	111.23
2	E	301	AM2	CC5-CC4-CC3	3.44	115.23	110.04
2	B	301	AM2	CC6-CC5-CC4	3.36	118.09	111.18
6	B	305	EPE	C7-N4-C3	3.24	119.53	111.23
6	E	305	EPE	C7-N4-C3	3.24	119.51	111.23
6	C	304	EPE	C5-N4-C3	3.23	116.09	108.83
6	D	305	EPE	C7-N4-C3	3.22	119.46	111.23
6	E	305	EPE	C7-N4-C5	3.09	119.15	111.23
6	F	303	EPE	C9-N1-C6	-3.03	103.49	111.23
2	D	301	AM2	CC5-CC4-CC3	2.99	114.55	110.04
6	A	308	EPE	C7-N4-C3	2.98	118.85	111.23
2	B	301	AM2	OA1-CC1-CC6	2.93	116.17	109.18
2	B	301	AM2	CC5-CC4-CC3	2.91	114.43	110.04
2	E	301	AM2	CC5-CC6-CC1	2.87	116.79	109.53
2	D	301	AM2	OA4-CA5-CA4	2.87	113.23	108.88
2	B	301	AM2	OA5-CA8-CA7	2.87	116.18	110.58
2	F	301	AM2	CC5-CC6-CC1	2.86	116.76	109.53
6	F	303	EPE	C6-C5-N4	-2.73	105.03	110.64
2	A	301	AM2	CC5-CC6-CC1	2.70	116.37	109.53
6	C	304	EPE	C7-N4-C3	2.70	118.13	111.23
2	A	301	AM2	CA1-OA4-CA5	-2.69	108.73	113.06
6	B	305	EPE	O2S-S-C10	2.64	110.09	106.92
2	F	301	AM2	CA1-OA4-CA5	-2.63	108.83	113.06
2	D	301	AM2	OA1-CC1-CC6	2.62	115.44	109.18
6	A	308	EPE	C7-N4-C5	2.58	117.84	111.23
6	A	308	EPE	O1S-S-C10	2.55	109.98	106.92
6	F	303	EPE	O2S-S-C10	-2.49	103.91	106.92
2	C	301	AM2	CA1-OA4-CA5	-2.49	109.05	113.06
6	A	308	EPE	O3S-S-C10	2.46	109.74	105.77
2	A	301	AM2	OA8-CB1-CB2	2.39	114.30	108.10
2	E	301	AM2	CA1-OA4-CA5	-2.35	109.27	113.06
6	C	304	EPE	C7-N4-C5	2.35	117.24	111.23
6	E	305	EPE	O2S-S-C10	2.33	109.72	106.92
2	D	301	AM2	CC5-CC6-CC1	2.31	115.38	109.53
2	A	301	AM2	OA1-CC1-CC6	2.28	114.61	109.18
6	F	303	EPE	C6-N1-C2	2.27	113.93	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	303	EPE	O2S-S-O1S	-2.26	106.11	113.95
6	A	308	EPE	C5-C6-N1	-2.26	106.01	110.64
2	B	301	AM2	CA8-OA5-CA4	2.22	118.05	113.69
2	F	301	AM2	OA8-CB1-CB2	2.21	113.83	108.10
6	E	305	EPE	O1S-S-C10	2.18	109.54	106.92
2	C	301	AM2	CC5-CC4-CC3	2.17	113.32	110.04
6	C	304	EPE	O3S-S-C10	2.15	109.24	105.77
2	B	301	AM2	OA8-CA8-OA5	-2.12	104.75	110.67
2	F	301	AM2	OA1-CC1-CC6	2.11	114.21	109.18
2	B	301	AM2	CC5-CC6-CC1	2.09	114.82	109.53
2	E	301	AM2	OA1-CC1-CC6	2.08	114.15	109.18
2	B	301	AM2	OA4-CA1-CA2	2.07	114.86	110.25
6	C	304	EPE	C6-N1-C2	2.05	113.45	108.83
6	D	305	EPE	O3S-S-C10	2.05	109.08	105.77
2	A	301	AM2	OA8-CA8-OA5	-2.04	104.96	110.67
6	B	305	EPE	O3S-S-C10	2.04	109.07	105.77
2	B	301	AM2	CA8-CA7-CA6	2.04	116.07	110.06

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	AM2	CB2-CB1-OA8-CA8
2	A	301	AM2	OB1-CB1-OA8-CA8
2	A	301	AM2	CC6-CC1-OA1-CA1
2	B	301	AM2	CA2-CA1-OA1-CC1
2	B	301	AM2	CA8-CA7-NA7-CA9
2	B	301	AM2	CA7-CA8-OA8-CB1
2	B	301	AM2	CB2-CB1-OA8-CA8
2	B	301	AM2	OB1-CB1-OA8-CA8
2	B	301	AM2	CC6-CC1-OA1-CA1
2	C	301	AM2	CA8-CA7-NA7-CA9
2	C	301	AM2	CB2-CB1-OA8-CA8
2	C	301	AM2	OB1-CB1-OA8-CA8
2	C	301	AM2	CC6-CC1-OA1-CA1
2	D	301	AM2	CA8-CA7-NA7-CA9
2	D	301	AM2	CA7-CA8-OA8-CB1
2	D	301	AM2	CB2-CB1-OA8-CA8
2	D	301	AM2	OB1-CB1-OA8-CA8
2	D	301	AM2	CC6-CC1-OA1-CA1
2	E	301	AM2	CA8-CA7-NA7-CA9
2	E	301	AM2	CB2-CB1-OA8-CA8

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Mol	Chain	Res	Type	Atoms
2	E	301	AM2	OB1-CB1-OA8-CA8
2	E	301	AM2	CC6-CC1-OA1-CA1
2	F	301	AM2	CA8-CA7-NA7-CA9
2	F	301	AM2	CB2-CB1-OA8-CA8
2	F	301	AM2	OB1-CB1-OA8-CA8
2	F	301	AM2	CC6-CC1-OA1-CA1
6	A	308	EPE	C9-C10-S-O2S
6	A	308	EPE	C9-C10-S-O3S
6	B	305	EPE	C8-C7-N4-C5
6	C	304	EPE	C10-C9-N1-C6
6	D	305	EPE	C8-C7-N4-C5
6	D	305	EPE	N4-C7-C8-O8
6	D	305	EPE	C9-C10-S-O2S
6	D	305	EPE	C9-C10-S-O3S
6	E	305	EPE	C10-C9-N1-C2
6	E	305	EPE	C10-C9-N1-C6
6	E	305	EPE	C9-C10-S-O1S
6	E	305	EPE	C9-C10-S-O2S
6	E	305	EPE	C9-C10-S-O3S
7	D	304	GOL	C1-C2-C3-O3
2	F	301	AM2	OB1-CB5-CB6-OB6
2	A	301	AM2	OB1-CB5-CB6-OB6
2	D	301	AM2	OB1-CB5-CB6-OB6
2	E	301	AM2	OB1-CB5-CB6-OB6
2	F	301	AM2	CB4-CB5-CB6-OB6
2	A	301	AM2	CB4-CB5-CB6-OB6
2	E	301	AM2	CB4-CB5-CB6-OB6
2	D	301	AM2	CB4-CB5-CB6-OB6
2	C	301	AM2	OB1-CB5-CB6-OB6
6	A	308	EPE	N4-C7-C8-O8
6	F	303	EPE	N4-C7-C8-O8
6	C	304	EPE	N4-C7-C8-O8
6	B	305	EPE	N4-C7-C8-O8
6	A	308	EPE	C8-C7-N4-C5
2	A	301	AM2	CA7-CA8-OA8-CB1
2	C	301	AM2	CA7-CA8-OA8-CB1
2	E	301	AM2	CA7-CA8-OA8-CB1
2	F	301	AM2	CA7-CA8-OA8-CB1
6	A	308	EPE	C10-C9-N1-C2
6	A	308	EPE	C10-C9-N1-C6
2	B	301	AM2	OA5-CA8-OA8-CB1
2	D	301	AM2	OA5-CA8-OA8-CB1

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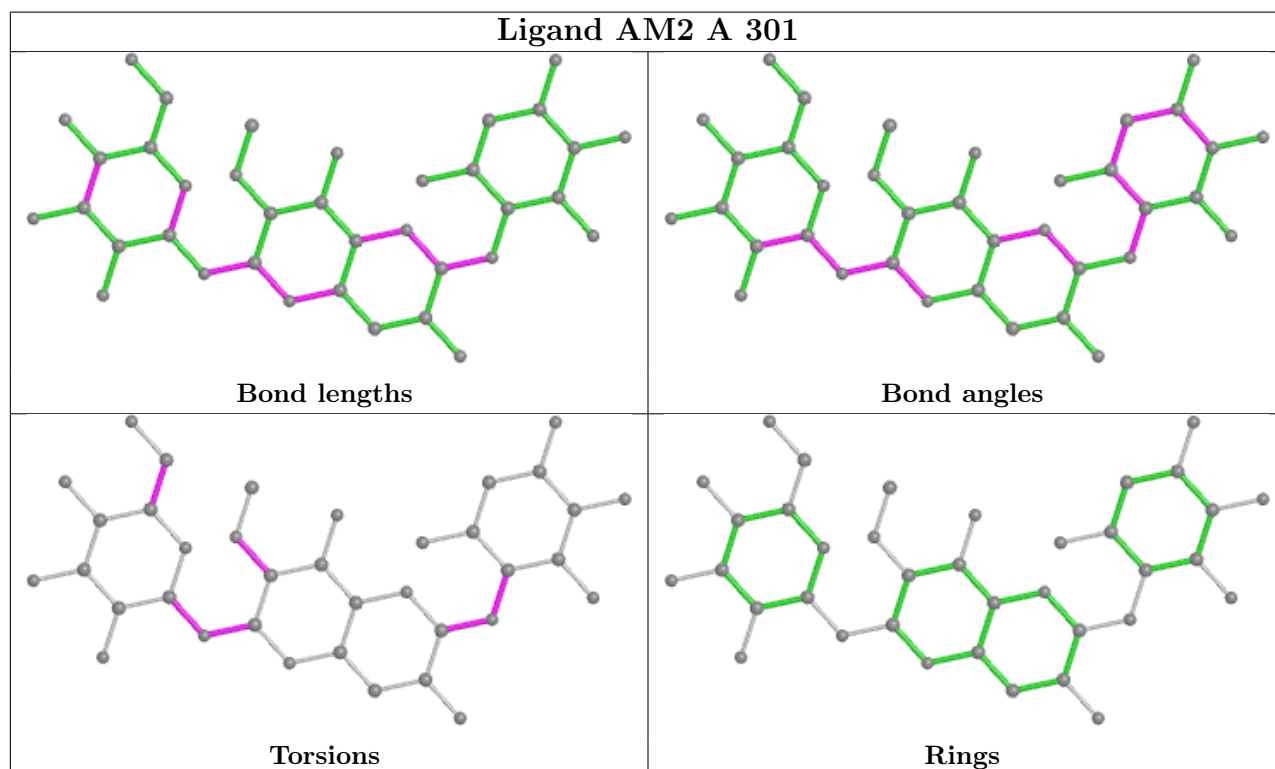
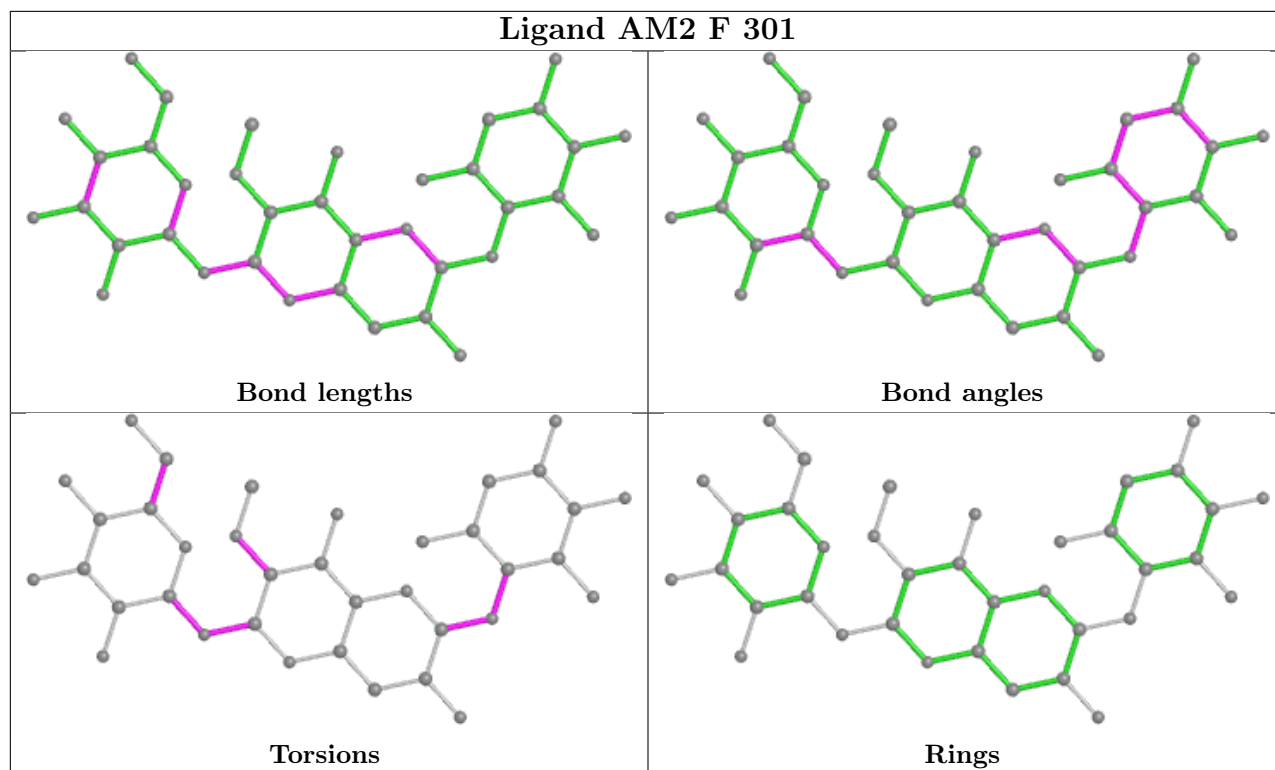
Mol	Chain	Res	Type	Atoms
2	E	301	AM2	OA5-CA8-OA8-CB1
2	A	301	AM2	OA5-CA8-OA8-CB1
2	F	301	AM2	OA5-CA8-OA8-CB1
7	D	304	GOL	O1-C1-C2-O2
7	D	304	GOL	O2-C2-C3-O3
2	C	301	AM2	CC2-CC1-OA1-CA1
2	F	301	AM2	CC2-CC1-OA1-CA1
6	A	308	EPE	C9-C10-S-O1S
6	D	305	EPE	C9-C10-S-O1S
2	A	301	AM2	CC2-CC1-OA1-CA1
6	C	304	EPE	C8-C7-N4-C3
2	C	301	AM2	CB4-CB5-CB6-OB6
2	C	301	AM2	OA5-CA8-OA8-CB1
2	E	301	AM2	CA2-CA1-OA1-CC1
2	F	301	AM2	CA2-CA1-OA1-CC1
6	B	305	EPE	C10-C9-N1-C2
6	B	305	EPE	C10-C9-N1-C6
2	E	301	AM2	CC2-CC1-OA1-CA1
2	A	301	AM2	CA8-CA7-NA7-CA9
7	D	304	GOL	O1-C1-C2-C3
2	B	301	AM2	OB1-CB5-CB6-OB6
4	A	304	EDO	O1-C1-C2-O2
2	A	301	AM2	CA2-CA1-OA1-CC1

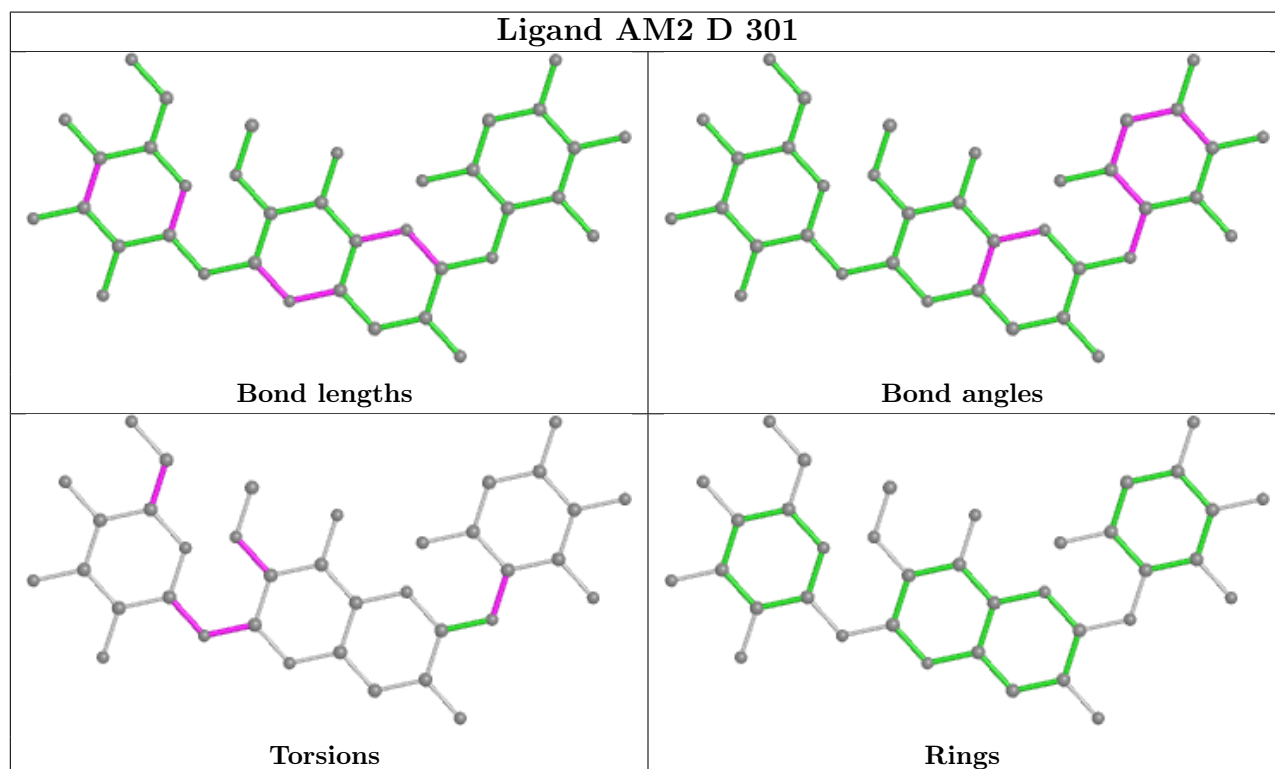
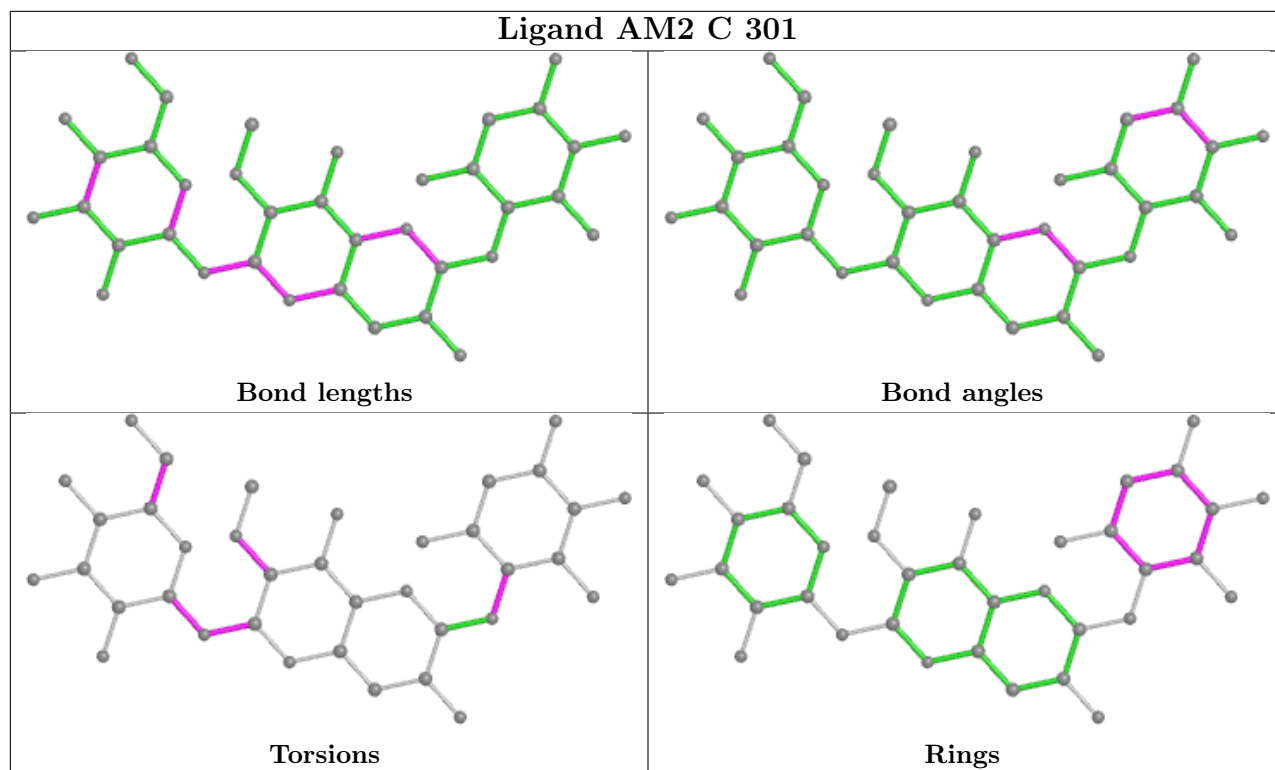
All (1) ring outliers are listed below:

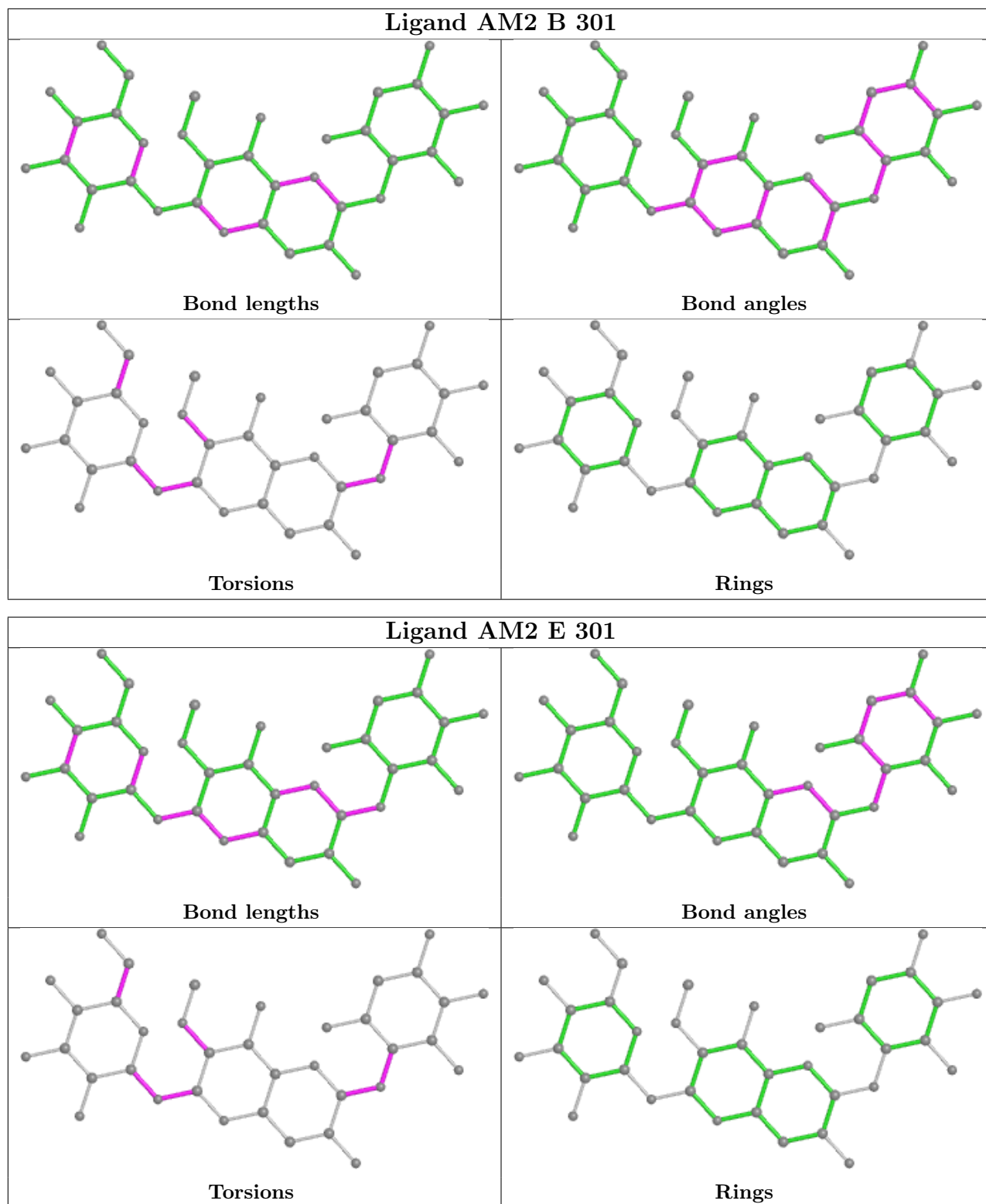
Mol	Chain	Res	Type	Atoms
2	C	301	AM2	CC1-CC2-CC3-CC4-CC5-CC6

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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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