



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:57 AM EDT

PDB ID : 6MN2
Title : Crystal structure of meta-AAC0038, an environmental aminoglycoside resistance enzyme, mutant H168A in abortive complex with sisomicin-CoA
Authors : Stogios, P.J.; Skarina, T.; Michalska, K.; Xu, Z.; Yim, V.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2018-10-01
Resolution : 2.74 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 2.74 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 7 unique types of molecules in this entry. The entry contains 4292 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.

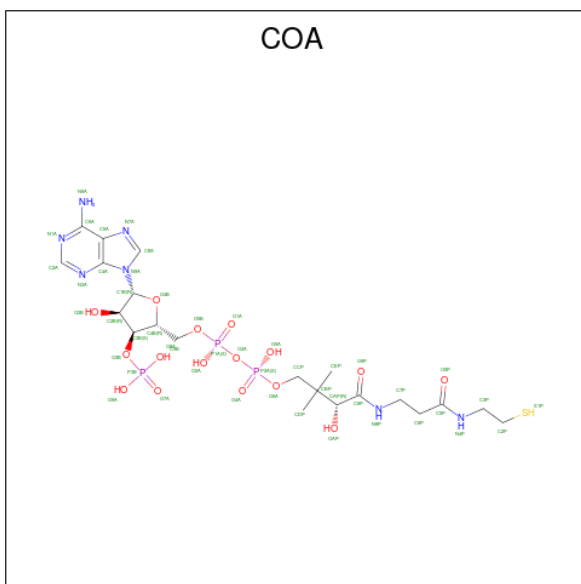
- Molecule 1 is a protein called Aminoglycoside N(3)-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	Total	C	N	O	S	0	0	0
			1996	1265	349	377	5			
1	B	259	Total	C	N	O	S	0	0	0
			1991	1262	348	376	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP A0A059X981
A	168	ALA	HIS	engineered mutation	UNP A0A059X981
B	1	VAL	-	expression tag	UNP A0A059X981
B	168	ALA	HIS	engineered mutation	UNP A0A059X981

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	79	Total 82	O 82	0	3
7	B	41	Total 43	O 43	0	2

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 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.75Å 127.75Å 95.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.20 – 2.74	Depositor
% Data completeness (in resolution range)	99.8 (29.20-2.74)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.76Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.249 , 0.270	Depositor
Wilson B-factor (Å ²)	37.9	Xtrriage
Anisotropy	0.155	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtrriage
Total number of atoms	4292	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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
3	SIS	B	302	2	28,33,33	1.75	5 (17%)	28,49,49	2.54	8 (28%)
2	COA	A	301	3	41,50,50	2.69	12 (29%)	52,75,75	1.52	5 (9%)
2	COA	B	301	3	41,50,50	2.70	12 (29%)	52,75,75	1.34	3 (5%)
5	PEG	A	306	-	6,6,6	1.05	0	5,5,5	2.03	1 (20%)
5	PEG	B	304	-	6,6,6	1.17	0	5,5,5	0.85	0
6	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SIS	A	302	2	28,33,33	1.63	3 (10%)	28,49,49	2.60	6 (21%)

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
3	SIS	B	302	2	-	0/9/65/65	0/3/3/3
2	COA	A	301	3	-	12/44/64/64	0/3/3/3
2	COA	B	301	3	-	6/44/64/64	0/3/3/3
5	PEG	A	306	-	-	1/4/4/4	-
5	PEG	B	304	-	-	1/4/4/4	-
3	SIS	A	302	2	-	0/9/65/65	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	COA	O4B-C1B	-8.01	1.29	1.41
2	B	301	COA	O4B-C1B	-7.78	1.30	1.41
2	B	301	COA	O4B-C4B	7.40	1.61	1.45
2	A	301	COA	O4B-C4B	7.00	1.60	1.45
2	A	301	COA	C3B-C4B	-6.99	1.34	1.52
2	B	301	COA	C3B-C4B	-6.87	1.34	1.52
3	B	302	SIS	C31-C41	-6.18	1.36	1.50
2	A	301	COA	C5P-N4P	5.65	1.46	1.33
3	A	302	SIS	C31-C41	-5.61	1.38	1.50
2	B	301	COA	C5P-N4P	5.59	1.46	1.33
2	A	301	COA	C9P-N8P	5.57	1.45	1.33
2	B	301	COA	C9P-N8P	5.40	1.45	1.33
3	A	302	SIS	C61-C51	-4.03	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	SIS	C61-C51	-3.46	1.40	1.48
2	A	301	COA	P3B-O3B	3.10	1.65	1.59
2	B	301	COA	P3B-O3B	2.96	1.64	1.59
2	A	301	COA	O2B-C2B	-2.92	1.36	1.43
2	B	301	COA	O2B-C2B	-2.89	1.36	1.43
2	A	301	COA	C5A-C4A	-2.82	1.33	1.40
2	B	301	COA	C6A-N6A	2.64	1.43	1.34
2	B	301	COA	C5A-C4A	-2.59	1.34	1.40
2	A	301	COA	C2B-C1B	2.51	1.57	1.53
2	B	301	COA	C2B-C1B	2.46	1.57	1.53
2	B	301	COA	C2A-N3A	2.44	1.36	1.32
2	A	301	COA	O9P-C9P	-2.34	1.18	1.23
2	B	301	COA	O9P-C9P	-2.27	1.18	1.23
2	A	301	COA	O5P-C5P	-2.25	1.18	1.23
2	A	301	COA	C2A-N3A	2.22	1.35	1.32
3	B	302	SIS	C52-C42	-2.16	1.46	1.52
3	B	302	SIS	C52-C62	-2.13	1.46	1.52
3	A	302	SIS	C52-C62	-2.11	1.46	1.52
3	B	302	SIS	O43-C43	-2.05	1.41	1.44

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	SIS	O11-C11-C21	-7.42	95.82	108.23
3	A	302	SIS	C93-N33-C33	7.41	125.18	114.38
3	B	302	SIS	O11-C11-C21	-6.75	96.95	108.23
3	B	302	SIS	C93-N33-C33	6.71	124.16	114.38
3	B	302	SIS	C11-O11-C42	-5.95	103.23	117.96
3	A	302	SIS	C11-O11-C42	-5.84	103.52	117.96
2	A	301	COA	N3A-C2A-N1A	-5.66	119.84	128.68
2	A	301	COA	C1B-N9A-C4A	-5.46	117.05	126.64
2	B	301	COA	N3A-C2A-N1A	-5.36	120.30	128.68
2	B	301	COA	C1B-N9A-C4A	-4.33	119.04	126.64
5	A	306	PEG	O2-C2-C1	3.49	125.38	110.07
3	B	302	SIS	O11-C42-C32	3.24	116.90	109.18
2	A	301	COA	C2P-C3P-N4P	-3.05	105.34	112.31
3	A	302	SIS	O53-C13-C23	2.92	114.53	110.04
3	B	302	SIS	O23-C23-C33	2.81	115.31	109.63
3	B	302	SIS	C13-O62-C62	2.73	124.72	117.96
3	B	302	SIS	O62-C62-C12	2.57	115.31	109.18
2	B	301	COA	C2P-C3P-N4P	-2.50	106.59	112.31
3	A	302	SIS	C13-O62-C62	2.35	123.77	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	COA	C7P-C6P-C5P	-2.31	108.52	112.36
2	A	301	COA	O6A-CCP-CBP	-2.29	106.86	110.55
3	B	302	SIS	C32-C22-C12	-2.19	106.68	111.18
3	A	302	SIS	O43-C43-C83	2.13	112.79	108.13

There are no chirality outliers.

All (20) torsion outliers are listed below:

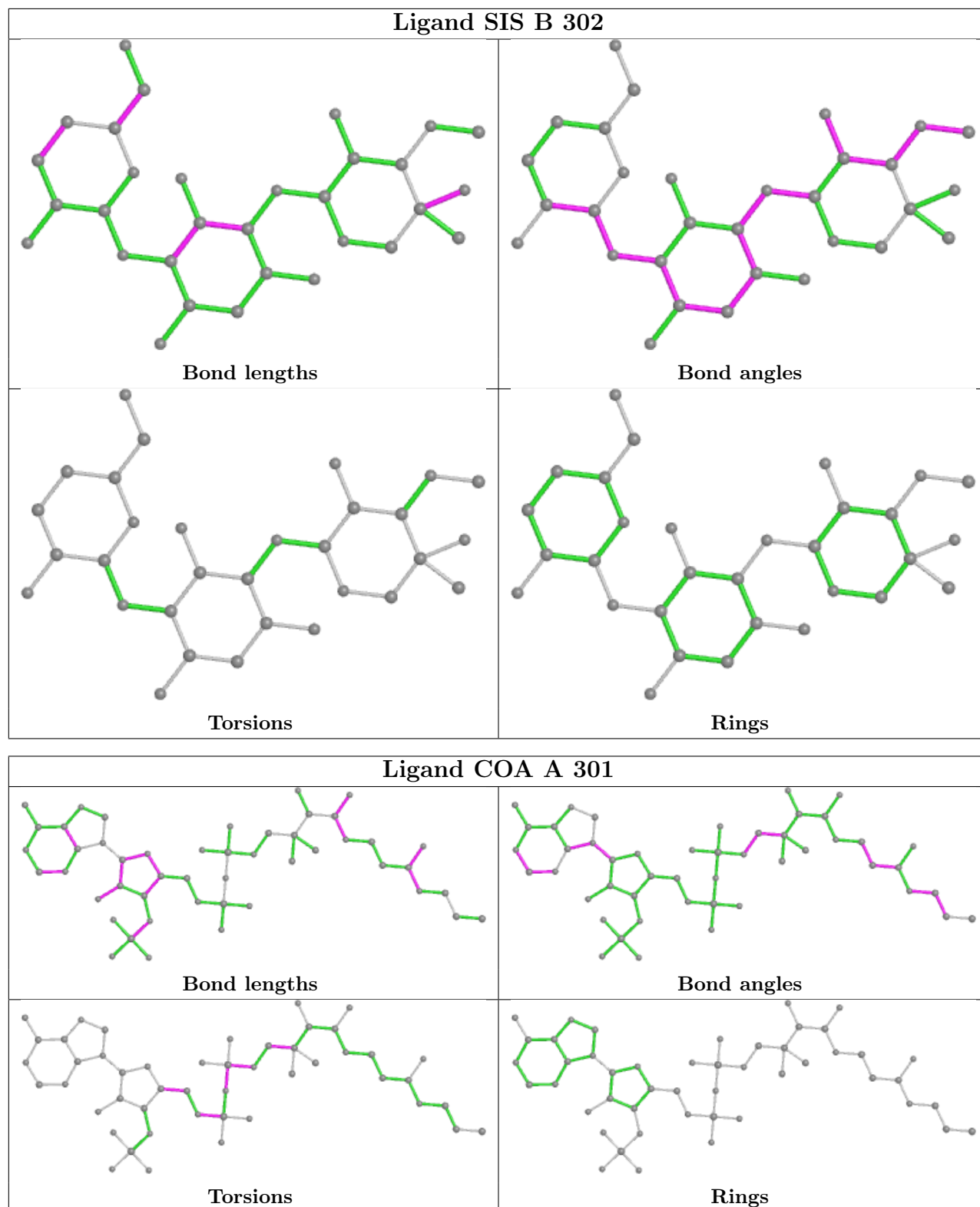
Mol	Chain	Res	Type	Atoms
2	A	301	COA	C3B-C4B-C5B-O5B
2	A	301	COA	O4B-C4B-C5B-O5B
2	A	301	COA	C5B-O5B-P1A-O1A
2	A	301	COA	C5B-O5B-P1A-O2A
2	A	301	COA	C5B-O5B-P1A-O3A
2	A	301	COA	CCP-O6A-P2A-O3A
2	A	301	COA	CAP-CBP-CCP-O6A
2	B	301	COA	P1A-O3A-P2A-O6A
2	B	301	COA	CCP-O6A-P2A-O5A
5	A	306	PEG	C1-C2-O2-C3
5	B	304	PEG	O1-C1-C2-O2
2	A	301	COA	CEP-CBP-CCP-O6A
2	A	301	COA	CDP-CBP-CCP-O6A
2	A	301	COA	P1A-O3A-P2A-O6A
2	B	301	COA	C3B-O3B-P3B-O9A
2	B	301	COA	CCP-O6A-P2A-O3A
2	A	301	COA	CCP-O6A-P2A-O4A
2	B	301	COA	CCP-O6A-P2A-O4A
2	B	301	COA	C2P-C3P-N4P-C5P
2	A	301	COA	P1A-O3A-P2A-O4A

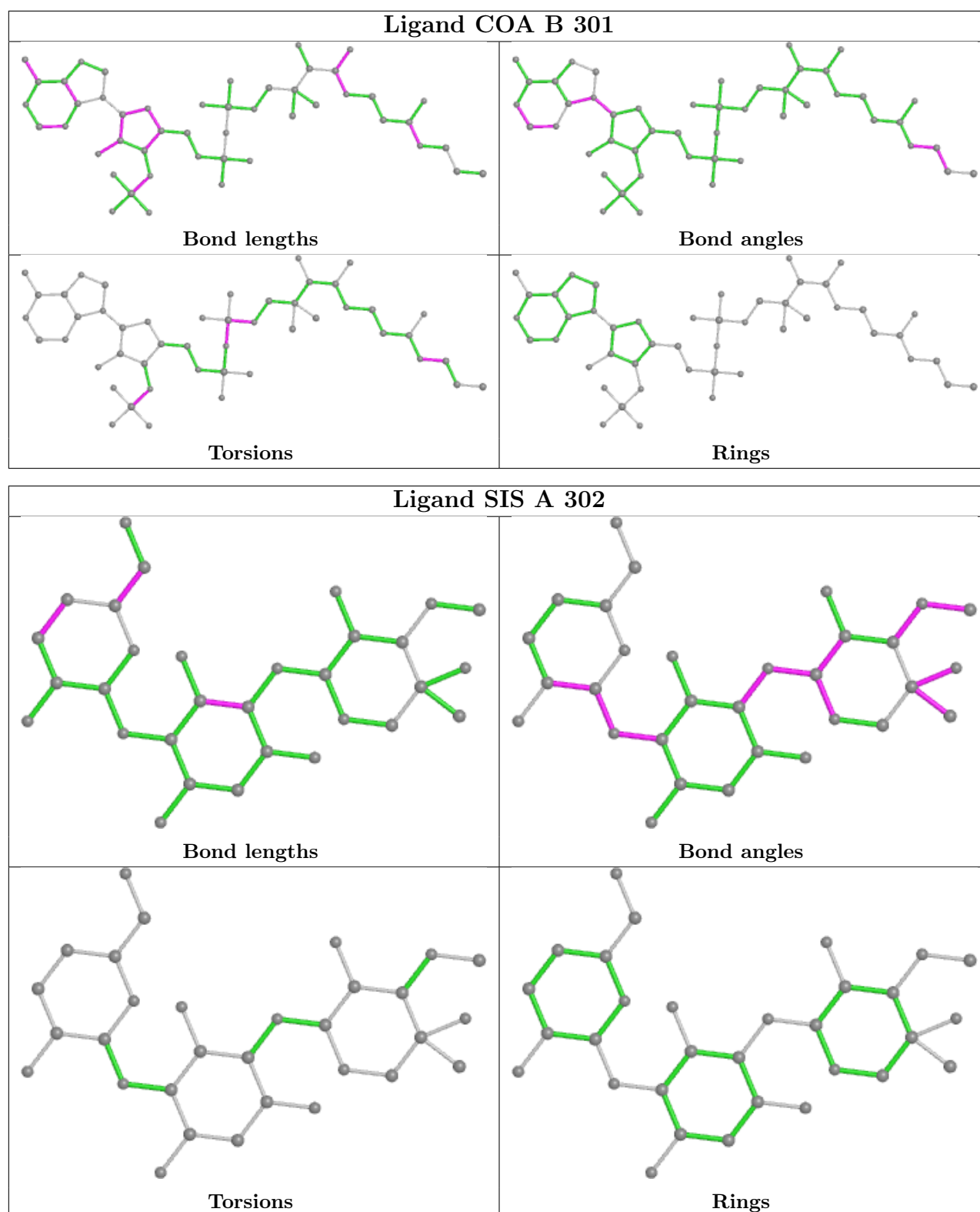
There are no ring outliers.

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.