Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 10:21 AM EDT

PDB ID	:	6MN0
Title	:	Crystal structure of meta-AAC0038, an environmental aminoglycoside resistance enzyme, H168A mutant in complex with acetyl-CoA
Authors	:	Stogios, P.J.; Skarina, T.; Zu, X.; Yim, V.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2018-10-01
Resolution	:	2.40 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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 14281 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.

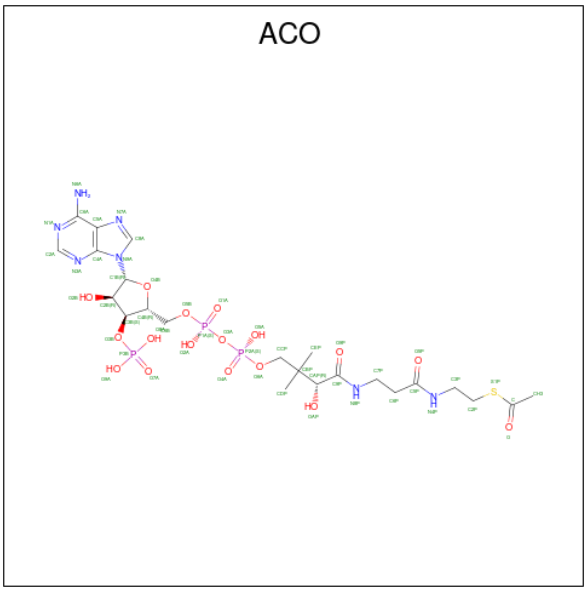
- Molecule 1 is a protein called Aminoglycoside N(3)-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	1	0
			2007	1271	352	379	5			
1	B	260	Total	C	N	O	S	0	1	0
			2007	1272	352	377	6			
1	C	261	Total	C	N	O	S	0	1	0
			2007	1271	350	381	5			
1	D	260	Total	C	N	O	S	0	0	0
			1996	1265	349	377	5			
1	E	260	Total	C	N	O	S	0	0	0
			2002	1268	352	377	5			
1	F	261	Total	C	N	O	S	0	1	0
			2014	1275	353	381	5			

There are 12 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
C	1	VAL	-	expression tag	UNP A0A059X981
C	168	ALA	HIS	engineered mutation	UNP A0A059X981
D	1	VAL	-	expression tag	UNP A0A059X981
D	168	ALA	HIS	engineered mutation	UNP A0A059X981
E	1	VAL	-	expression tag	UNP A0A059X981
E	168	ALA	HIS	engineered mutation	UNP A0A059X981
F	1	VAL	-	expression tag	UNP A0A059X981
F	168	ALA	HIS	engineered mutation	UNP A0A059X981

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).

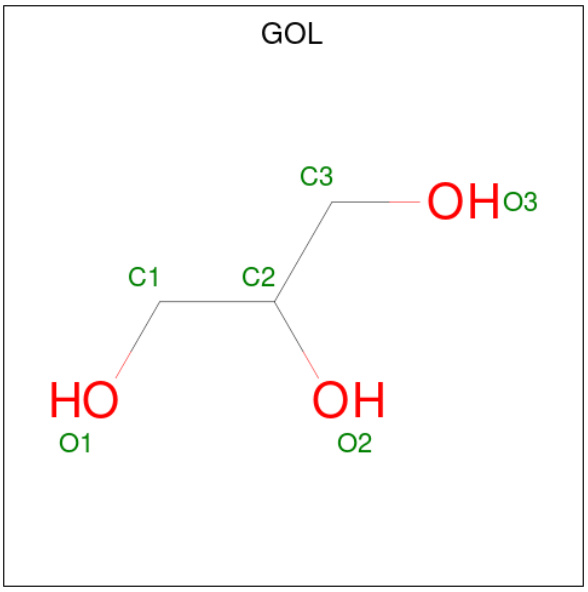


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

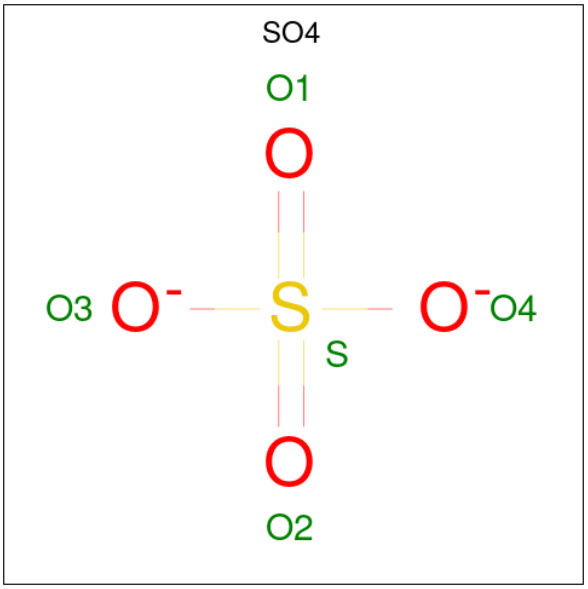
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

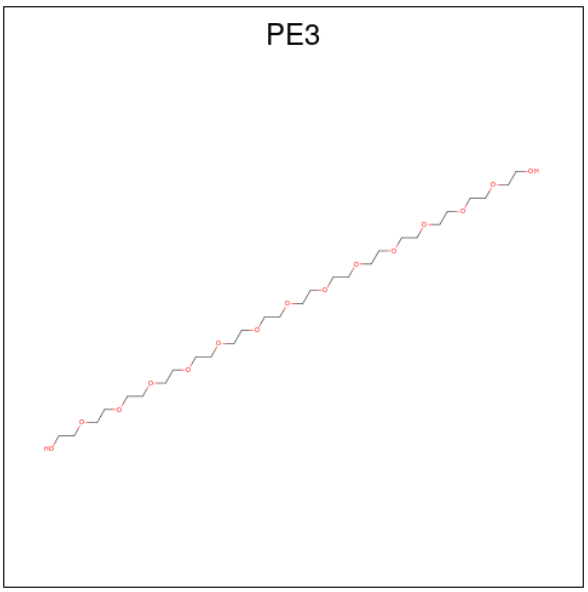
- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1

,41-DIOL (three-letter code: PE3) (formula: $C_{28}H_{58}O_{15}$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	281	Total O 295 295	0	13
7	B	278	Total O 291 291	0	13
7	C	312	Total O 327 327	0	15

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	253	Total O 260 260	0	7
7	E	254	Total O 262 262	0	8
7	F	267	Total O 271 271	0	4

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	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.08Å 159.62Å 143.32Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	24.93 – 2.40	Depositor
% Data completeness (in resolution range)	99.5 (24.93-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.39Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, R_{free}	0.178 , 0.208	Depositor
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.262	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14281	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 43 ligands modelled in this entry, 3 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
5	SO4	D	305	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	F	305	-	4,4,4	0.14	0	6,6,6	0.09	0
4	GOL	A	303	-	5,5,5	1.01	0	5,5,5	1.05	0
6	PE3	E	309	-	9,9,42	0.73	0	8,8,41	2.06	4 (50%)
6	PE3	B	305	-	12,12,42	0.62	0	11,11,41	1.90	2 (18%)
2	ACO	A	301	-	45,53,53	1.73	5 (11%)	56,79,79	4.79	21 (37%)
4	GOL	D	304	-	5,5,5	0.92	0	5,5,5	0.94	0
5	SO4	E	307	-	4,4,4	0.16	0	6,6,6	0.42	0
6	PE3	B	304	-	12,12,42	1.11	1 (8%)	11,11,41	2.52	6 (54%)
4	GOL	D	303	-	5,5,5	1.07	0	5,5,5	0.89	0
5	SO4	A	305	-	4,4,4	0.32	0	6,6,6	0.05	0
5	SO4	F	303	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	306	-	4,4,4	0.14	0	6,6,6	0.06	0
6	PE3	A	309	-	12,12,42	0.39	0	11,11,41	1.51	2 (18%)
5	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	306	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	E	304	-	4,4,4	0.17	0	6,6,6	0.65	0
4	GOL	D	302	-	5,5,5	0.94	0	5,5,5	0.97	0
5	SO4	F	304	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	E	306	-	4,4,4	0.14	0	6,6,6	0.04	0
6	PE3	A	308	-	9,9,42	0.54	0	8,8,41	0.79	0
2	ACO	B	301	-	45,53,53	2.31	12 (26%)	56,79,79	4.53	22 (39%)
5	SO4	A	304	-	4,4,4	0.30	0	6,6,6	0.64	0
5	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	E	308	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	E	303	-	4,4,4	0.14	0	6,6,6	0.04	0
4	GOL	E	302	-	5,5,5	1.00	0	5,5,5	0.79	0
5	SO4	D	306	-	4,4,4	0.14	0	6,6,6	0.06	0
6	PE3	F	307	-	12,12,42	0.46	0	11,11,41	1.83	3 (27%)
5	SO4	C	304	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	F	306	-	4,4,4	0.14	0	6,6,6	0.05	0
6	PE3	C	307	-	12,12,42	0.59	0	11,11,41	1.29	2 (18%)
2	ACO	E	301	-	45,53,53	2.11	8 (17%)	56,79,79	3.27	15 (26%)
6	PE3	A	307	-	12,12,42	0.45	0	11,11,41	2.07	4 (36%)
5	SO4	B	303	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	E	305	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	B	302	-	4,4,4	0.13	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ACO	F	301	-	45,53,53	1.57	5 (11%)	56,79,79	4.57	19 (33%)
2	ACO	D	301	-	45,53,53	1.53	5 (11%)	56,79,79	4.74	20 (35%)
2	ACO	C	301	-	45,53,53	1.55	5 (11%)	56,79,79	4.77	18 (32%)

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	GOL	A	303	-	-	2/4/4/4	-
6	PE3	E	309	-	-	3/7/7/40	-
6	PE3	B	305	-	-	2/10/10/40	-
2	ACO	A	301	-	-	12/47/67/67	0/3/3/3
4	GOL	D	304	-	-	4/4/4/4	-
6	PE3	B	304	-	-	5/10/10/40	-
4	GOL	D	303	-	-	1/4/4/4	-
6	PE3	A	309	-	-	1/10/10/40	-
4	GOL	D	302	-	-	2/4/4/4	-
6	PE3	A	308	-	-	0/7/7/40	-
2	ACO	B	301	-	-	9/47/67/67	0/3/3/3
6	PE3	F	307	-	-	2/10/10/40	-
4	GOL	E	302	-	-	0/4/4/4	-
6	PE3	C	307	-	-	2/10/10/40	-
2	ACO	E	301	-	-	5/47/67/67	0/3/3/3
6	PE3	A	307	-	-	2/10/10/40	-
2	ACO	F	301	-	-	9/47/67/67	0/3/3/3
2	ACO	D	301	-	-	12/47/67/67	0/3/3/3
2	ACO	C	301	-	-	9/47/67/67	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ACO	O4B-C1B	7.43	1.51	1.41
2	A	301	ACO	O4B-C1B	7.36	1.51	1.41
2	B	301	ACO	C2B-C3B	6.96	1.68	1.52
2	E	301	ACO	C2B-C3B	6.16	1.66	1.52
2	C	301	ACO	O4B-C1B	5.92	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	ACO	O4B-C1B	5.91	1.49	1.41
2	F	301	ACO	O4B-C1B	5.63	1.48	1.41
2	E	301	ACO	O4B-C1B	5.58	1.48	1.41
2	E	301	ACO	C2B-C1B	-5.57	1.45	1.53
2	E	301	ACO	C3B-C4B	-5.12	1.39	1.52
2	B	301	ACO	C2A-N3A	5.02	1.40	1.32
2	B	301	ACO	C3B-C4B	-5.02	1.39	1.52
2	A	301	ACO	C2A-N3A	5.00	1.40	1.32
2	F	301	ACO	C2A-N3A	4.96	1.40	1.32
2	D	301	ACO	C2A-N3A	4.82	1.39	1.32
2	E	301	ACO	C2A-N3A	4.78	1.39	1.32
2	C	301	ACO	C2A-N3A	4.57	1.39	1.32
2	B	301	ACO	C2B-C1B	-4.36	1.47	1.53
2	F	301	ACO	C2A-N1A	3.17	1.39	1.33
2	A	301	ACO	C2A-N1A	3.16	1.39	1.33
2	C	301	ACO	C2A-N1A	3.14	1.39	1.33
2	B	301	ACO	C2A-N1A	3.10	1.39	1.33
2	D	301	ACO	C2A-N1A	3.08	1.39	1.33
2	E	301	ACO	C2A-N1A	3.00	1.39	1.33
2	C	301	ACO	C5A-C4A	-2.84	1.33	1.40
2	A	301	ACO	C5A-C4A	-2.83	1.33	1.40
2	D	301	ACO	C5A-C4A	-2.82	1.33	1.40
2	B	301	ACO	O2B-C2B	2.79	1.49	1.43
2	F	301	ACO	C5A-C4A	-2.74	1.33	1.40
6	B	304	PE3	O34-C35	2.50	1.52	1.42
2	A	301	ACO	C6A-C5A	-2.43	1.34	1.43
2	D	301	ACO	C6A-C5A	-2.43	1.34	1.43
2	F	301	ACO	C6A-C5A	-2.41	1.34	1.43
2	C	301	ACO	C6A-C5A	-2.39	1.34	1.43
2	B	301	ACO	O4B-C4B	2.37	1.50	1.45
2	B	301	ACO	C5A-C4A	-2.37	1.34	1.40
2	B	301	ACO	P1A-O5B	2.35	1.68	1.59
2	B	301	ACO	C6A-C5A	-2.30	1.34	1.43
2	B	301	ACO	C5B-C4B	2.27	1.58	1.51
2	E	301	ACO	C5A-C4A	-2.26	1.34	1.40
2	E	301	ACO	C6A-C5A	-2.21	1.35	1.43

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	ACO	O4B-C4B-C3B	-16.50	69.50	104.87
2	D	301	ACO	O4B-C4B-C3B	-16.04	70.50	104.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	ACO	O4B-C4B-C3B	-16.00	70.59	104.87
2	A	301	ACO	O4B-C1B-C2B	-15.98	83.58	106.93
2	B	301	ACO	O4B-C1B-C2B	-15.90	83.69	106.93
2	F	301	ACO	O4B-C4B-C3B	-15.81	70.99	104.87
2	E	301	ACO	O4B-C1B-C2B	-15.28	84.59	106.93
2	B	301	ACO	CEP-CBP-CCP	-14.89	83.95	108.23
2	C	301	ACO	CEP-CBP-CCP	-14.77	84.14	108.23
2	D	301	ACO	CEP-CBP-CCP	-14.61	84.40	108.23
2	F	301	ACO	CDP-CBP-CCP	-14.23	85.02	108.23
2	F	301	ACO	O4B-C1B-C2B	-14.22	86.15	106.93
2	D	301	ACO	CDP-CBP-CCP	-14.14	85.16	108.23
2	A	301	ACO	CEP-CBP-CCP	-14.14	85.17	108.23
2	C	301	ACO	CDP-CBP-CCP	-14.04	85.33	108.23
2	F	301	ACO	CEP-CBP-CCP	-13.90	85.56	108.23
2	A	301	ACO	CDP-CBP-CCP	-13.82	85.69	108.23
2	D	301	ACO	O4B-C1B-C2B	-13.75	86.84	106.93
2	C	301	ACO	O4B-C1B-C2B	-13.64	86.99	106.93
2	B	301	ACO	CDP-CBP-CCP	-13.46	86.28	108.23
2	C	301	ACO	C1B-N9A-C4A	-11.98	105.59	126.64
2	D	301	ACO	C1B-N9A-C4A	-9.83	109.36	126.64
2	A	301	ACO	C1B-N9A-C4A	-9.35	110.20	126.64
2	E	301	ACO	C2B-C3B-C4B	-8.50	88.16	103.22
2	B	301	ACO	C2B-C3B-C4B	-7.74	89.50	103.22
2	F	301	ACO	C1B-N9A-C4A	-7.60	113.28	126.64
2	B	301	ACO	C1B-N9A-C4A	-7.23	113.94	126.64
2	C	301	ACO	N3A-C2A-N1A	-7.07	117.62	128.68
2	E	301	ACO	C5B-C4B-C3B	7.06	137.78	114.40
2	B	301	ACO	C5B-C4B-C3B	7.00	137.60	114.40
2	D	301	ACO	N3A-C2A-N1A	-7.00	117.74	128.68
2	A	301	ACO	N3A-C2A-N1A	-7.00	117.75	128.68
2	F	301	ACO	N3A-C2A-N1A	-6.74	118.14	128.68
2	E	301	ACO	C1B-N9A-C4A	-6.70	114.88	126.64
2	B	301	ACO	N3A-C2A-N1A	-6.58	118.40	128.68
2	E	301	ACO	N3A-C2A-N1A	-6.57	118.42	128.68
2	B	301	ACO	CEP-CBP-CAP	6.53	120.14	108.82
2	F	301	ACO	CEP-CBP-CAP	6.49	120.08	108.82
2	A	301	ACO	CEP-CBP-CDP	6.43	122.27	109.17
2	C	301	ACO	CEP-CBP-CDP	6.32	122.04	109.17
2	B	301	ACO	CEP-CBP-CDP	6.28	121.97	109.17
2	C	301	ACO	CEP-CBP-CAP	6.21	119.59	108.82
2	F	301	ACO	CEP-CBP-CDP	6.21	121.82	109.17
2	D	301	ACO	CEP-CBP-CDP	6.17	121.73	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	ACO	CEP-CBP-CAP	6.10	119.39	108.82
2	F	301	ACO	C2B-C3B-C4B	-6.00	92.58	103.22
2	A	301	ACO	CEP-CBP-CAP	5.95	119.13	108.82
2	C	301	ACO	C2B-C3B-C4B	-5.63	93.25	103.22
2	B	301	ACO	O3B-C3B-C4B	-5.56	89.97	110.08
2	D	301	ACO	CDP-CBP-CAP	5.53	118.41	108.82
2	A	301	ACO	CDP-CBP-CAP	5.51	118.37	108.82
2	B	301	ACO	C3B-C2B-C1B	5.47	112.01	99.89
2	E	301	ACO	O3B-C3B-C4B	-5.42	90.47	110.08
2	D	301	ACO	C2B-C3B-C4B	-5.32	93.80	103.22
2	C	301	ACO	CDP-CBP-CAP	5.30	118.02	108.82
6	B	304	PE3	O40-C39-C38	5.23	133.97	110.39
2	E	301	ACO	C3B-C2B-C1B	5.20	111.42	99.89
2	F	301	ACO	CDP-CBP-CAP	5.20	117.83	108.82
2	B	301	ACO	O5B-C5B-C4B	5.12	126.63	108.99
2	A	301	ACO	C2B-C3B-C4B	-5.09	94.21	103.22
2	B	301	ACO	CDP-CBP-CAP	5.06	117.60	108.82
2	D	301	ACO	C6P-C7P-N8P	-4.84	102.12	111.90
2	E	301	ACO	O5B-C5B-C4B	4.59	124.80	108.99
2	D	301	ACO	C3P-N4P-C5P	-4.51	114.45	122.84
6	B	305	PE3	C33-O34-C35	-4.48	93.88	113.29
2	E	301	ACO	O3B-P3B-O7A	-3.91	94.30	109.39
6	B	304	PE3	O37-C38-C39	3.89	127.94	110.39
6	A	307	PE3	O37-C36-C35	-3.86	92.97	110.39
2	C	301	ACO	C6P-C7P-N8P	-3.84	104.14	111.90
6	F	307	PE3	O40-C39-C38	3.77	127.41	110.39
2	B	301	ACO	O3B-P3B-O7A	-3.76	94.87	109.39
2	A	301	ACO	C6P-C7P-N8P	-3.61	104.60	111.90
2	B	301	ACO	C6P-C7P-N8P	-3.59	104.64	111.90
2	F	301	ACO	C6P-C7P-N8P	-3.40	105.02	111.90
6	F	307	PE3	C39-O40-C41	-3.23	99.28	113.29
6	A	307	PE3	C33-O34-C35	-3.18	99.51	113.29
6	E	309	PE3	O34-C35-C36	-2.99	96.90	110.39
6	A	307	PE3	C39-O40-C41	-2.99	100.35	113.29
2	A	301	ACO	C5B-C4B-C3B	-2.94	104.67	114.40
6	E	309	PE3	O37-C36-C35	2.88	123.40	110.39
2	B	301	ACO	C3P-N4P-C5P	-2.88	117.48	122.84
2	B	301	ACO	O2B-C2B-C3B	2.87	119.31	111.17
2	A	301	ACO	O2B-C2B-C3B	2.82	119.18	111.17
6	E	309	PE3	O34-C33-C32	2.79	122.34	110.07
2	D	301	ACO	O3B-P3B-O7A	-2.78	98.65	109.39
2	D	301	ACO	C2P-C3P-N4P	2.72	118.13	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	309	PE3	O40-C39-C38	2.65	122.36	110.39
2	A	301	ACO	O3B-P3B-O7A	-2.62	99.28	109.39
6	B	304	PE3	O34-C33-C32	2.62	121.57	110.07
2	C	301	ACO	O3B-P3B-O7A	-2.60	99.37	109.39
2	F	301	ACO	C5B-C4B-C3B	-2.56	105.92	114.40
2	E	301	ACO	C4A-C5A-N7A	-2.56	106.73	109.40
2	C	301	ACO	C4A-C5A-N7A	-2.55	106.74	109.40
2	C	301	ACO	C5B-C4B-C3B	-2.54	105.98	114.40
2	E	301	ACO	C3P-N4P-C5P	-2.54	118.12	122.84
2	D	301	ACO	C5B-C4B-C3B	-2.51	106.08	114.40
6	A	307	PE3	C36-O37-C38	-2.51	102.42	113.29
2	E	301	ACO	O5A-P2A-O4A	2.47	124.46	112.24
6	B	304	PE3	O37-C36-C35	2.43	121.33	110.39
6	C	307	PE3	O34-C35-C36	2.41	121.25	110.39
2	E	301	ACO	O6A-P2A-O4A	2.40	118.45	109.07
2	D	301	ACO	C4A-C5A-N7A	-2.40	106.90	109.40
2	A	301	ACO	O6A-P2A-O4A	2.39	118.42	109.07
2	B	301	ACO	C4A-C5A-N7A	-2.36	106.94	109.40
2	D	301	ACO	O5A-P2A-O6A	2.35	118.65	107.75
2	A	301	ACO	C5A-C6A-N6A	-2.34	116.79	120.35
2	D	301	ACO	O5A-P2A-O4A	2.34	123.80	112.24
2	F	301	ACO	O3B-P3B-O7A	-2.31	100.49	109.39
6	B	305	PE3	C36-O37-C38	-2.31	103.30	113.29
2	C	301	ACO	O5A-P2A-O6A	2.30	118.43	107.75
2	C	301	ACO	O5A-P2A-O4A	2.30	123.59	112.24
2	A	301	ACO	C4A-C5A-N7A	-2.29	107.01	109.40
2	F	301	ACO	C4A-C5A-N7A	-2.29	107.01	109.40
6	E	309	PE3	C33-O34-C35	-2.28	103.43	113.29
6	B	304	PE3	O31-C32-C33	-2.27	98.65	111.81
2	F	301	ACO	O5A-P2A-O6A	2.26	118.26	107.75
2	B	301	ACO	O5A-P2A-O4A	2.26	123.42	112.24
2	A	301	ACO	O5A-P2A-O4A	2.26	123.41	112.24
2	E	301	ACO	C6P-C7P-N8P	-2.26	107.34	111.90
2	B	301	ACO	O5A-P2A-O6A	2.25	118.20	107.75
2	F	301	ACO	C5A-C6A-N6A	-2.24	116.95	120.35
2	F	301	ACO	O5A-P2A-O4A	2.23	123.24	112.24
2	D	301	ACO	C5A-C6A-N6A	-2.21	116.99	120.35
6	B	304	PE3	C36-O37-C38	-2.21	103.70	113.29
6	F	307	PE3	C36-O37-C38	-2.21	103.73	113.29
2	A	301	ACO	O2B-C2B-C1B	2.20	118.97	110.85
2	B	301	ACO	O6A-P2A-O4A	2.14	117.43	109.07
2	C	301	ACO	O9A-P3B-O8A	2.13	115.77	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	ACO	O6A-P2A-O4A	2.12	117.35	109.07
2	C	301	ACO	C5A-C6A-N6A	-2.11	117.15	120.35
2	B	301	ACO	O9A-P3B-O8A	2.08	115.59	107.64
6	C	307	PE3	C36-O37-C38	-2.08	104.28	113.29
2	A	301	ACO	O5B-C5B-C4B	2.07	116.13	108.99
2	F	301	ACO	O9A-P3B-O8A	2.07	115.53	107.64
2	A	301	ACO	O5A-P2A-O6A	2.06	117.30	107.75
6	A	309	PE3	C36-O37-C38	-2.05	104.39	113.29
2	E	301	ACO	O9A-P3B-O8A	2.01	115.30	107.64
2	D	301	ACO	O9A-P3B-O8A	2.00	115.29	107.64

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ACO	CCP-O6A-P2A-O5A
2	A	301	ACO	C9P-CAP-CBP-CDP
2	A	301	ACO	OAP-CAP-CBP-CEP
2	A	301	ACO	C9P-CAP-CBP-CEP
2	B	301	ACO	CCP-O6A-P2A-O5A
2	B	301	ACO	C9P-CAP-CBP-CDP
2	B	301	ACO	OAP-CAP-CBP-CEP
2	B	301	ACO	C9P-CAP-CBP-CEP
2	B	301	ACO	C3P-C2P-S1P-C
2	C	301	ACO	CCP-O6A-P2A-O5A
2	C	301	ACO	C9P-CAP-CBP-CDP
2	C	301	ACO	OAP-CAP-CBP-CEP
2	C	301	ACO	C9P-CAP-CBP-CEP
2	D	301	ACO	CCP-O6A-P2A-O5A
2	D	301	ACO	C9P-CAP-CBP-CDP
2	D	301	ACO	OAP-CAP-CBP-CEP
2	D	301	ACO	C9P-CAP-CBP-CEP
2	D	301	ACO	C3P-C2P-S1P-C
2	D	301	ACO	O-C-S1P-C2P
2	D	301	ACO	CH3-C-S1P-C2P
2	E	301	ACO	CCP-O6A-P2A-O5A
2	F	301	ACO	CCP-O6A-P2A-O5A
2	F	301	ACO	C9P-CAP-CBP-CDP
2	F	301	ACO	OAP-CAP-CBP-CEP
2	F	301	ACO	C9P-CAP-CBP-CEP
4	D	302	GOL	O1-C1-C2-O2
4	D	302	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	D	304	GOL	O1-C1-C2-C3
4	D	304	GOL	C1-C2-C3-O3
2	B	301	ACO	O4B-C4B-C5B-O5B
2	E	301	ACO	O4B-C4B-C5B-O5B
4	D	304	GOL	O2-C2-C3-O3
2	A	301	ACO	O4B-C4B-C5B-O5B
2	C	301	ACO	O4B-C4B-C5B-O5B
2	D	301	ACO	O4B-C4B-C5B-O5B
2	F	301	ACO	O4B-C4B-C5B-O5B
2	A	301	ACO	C4B-C3B-O3B-P3B
2	B	301	ACO	C4B-C3B-O3B-P3B
2	C	301	ACO	C2B-C3B-O3B-P3B
2	C	301	ACO	C4B-C3B-O3B-P3B
2	D	301	ACO	C2B-C3B-O3B-P3B
2	E	301	ACO	C4B-C3B-O3B-P3B
2	F	301	ACO	C2B-C3B-O3B-P3B
6	B	304	PE3	C39-C38-O37-C36
4	D	304	GOL	O1-C1-C2-O2
2	F	301	ACO	C4B-C3B-O3B-P3B
6	F	307	PE3	C36-C35-O34-C33
2	A	301	ACO	OAP-CAP-CBP-CDP
2	B	301	ACO	OAP-CAP-CBP-CDP
2	C	301	ACO	OAP-CAP-CBP-CDP
2	D	301	ACO	OAP-CAP-CBP-CDP
2	F	301	ACO	OAP-CAP-CBP-CDP
6	E	309	PE3	C39-C38-O37-C36
6	A	309	PE3	C38-C39-O40-C41
2	E	301	ACO	C3P-C2P-S1P-C
2	A	301	ACO	C2B-C3B-O3B-P3B
2	D	301	ACO	C4B-C3B-O3B-P3B
6	A	307	PE3	C35-C36-O37-C38
4	A	303	GOL	O1-C1-C2-O2
6	F	307	PE3	C42-C41-O40-C39
6	B	304	PE3	C32-C33-O34-C35
2	F	301	ACO	C2P-C3P-N4P-C5P
4	D	303	GOL	O2-C2-C3-O3
6	C	307	PE3	C39-C38-O37-C36
2	A	301	ACO	C3P-C2P-S1P-C
6	B	304	PE3	C35-C36-O37-C38
2	A	301	ACO	C2P-C3P-N4P-C5P
6	B	304	PE3	O34-C35-C36-O37
6	C	307	PE3	C42-C41-O40-C39

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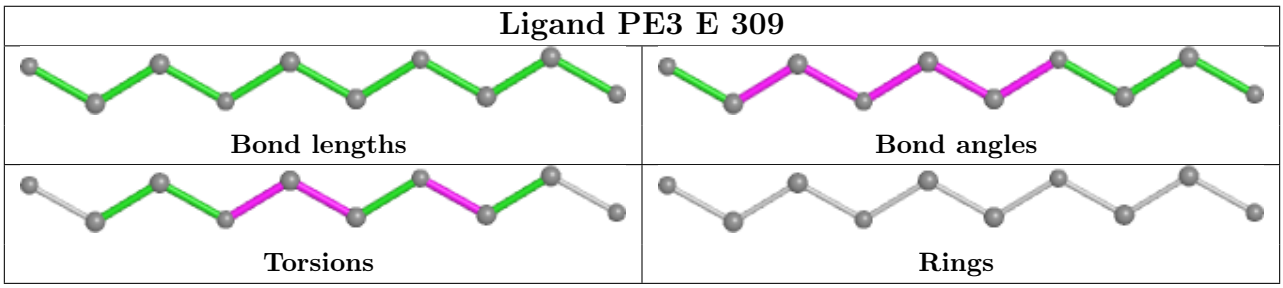
Mol	Chain	Res	Type	Atoms
2	A	301	ACO	C3B-O3B-P3B-O9A
2	A	301	ACO	CCP-O6A-P2A-O3A
2	B	301	ACO	CCP-O6A-P2A-O3A
2	C	301	ACO	CCP-O6A-P2A-O3A
2	D	301	ACO	CCP-O6A-P2A-O3A
2	E	301	ACO	CCP-O6A-P2A-O3A
6	E	309	PE3	O34-C35-C36-O37
6	B	304	PE3	C38-C39-O40-C41
6	E	309	PE3	C36-C35-O34-C33
6	B	305	PE3	C36-C35-O34-C33
4	A	303	GOL	O1-C1-C2-C3
6	A	307	PE3	O34-C35-C36-O37
6	B	305	PE3	O34-C35-C36-O37

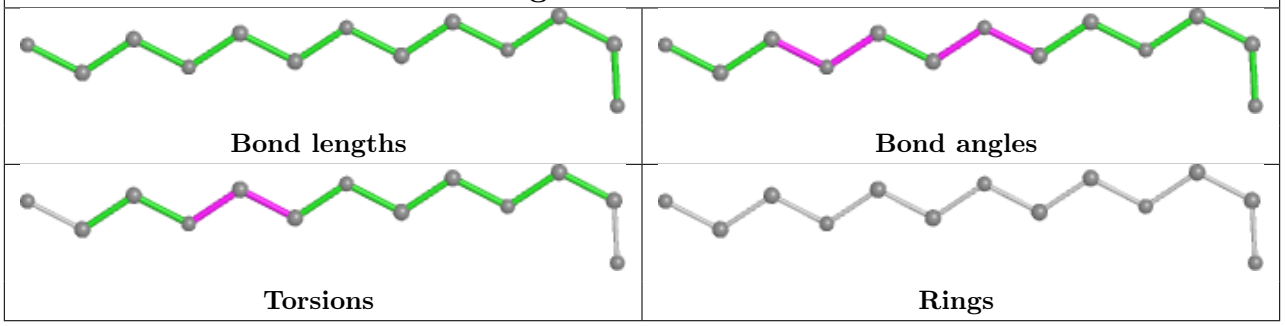
There are no ring outliers.

No monomer is involved in short contacts.

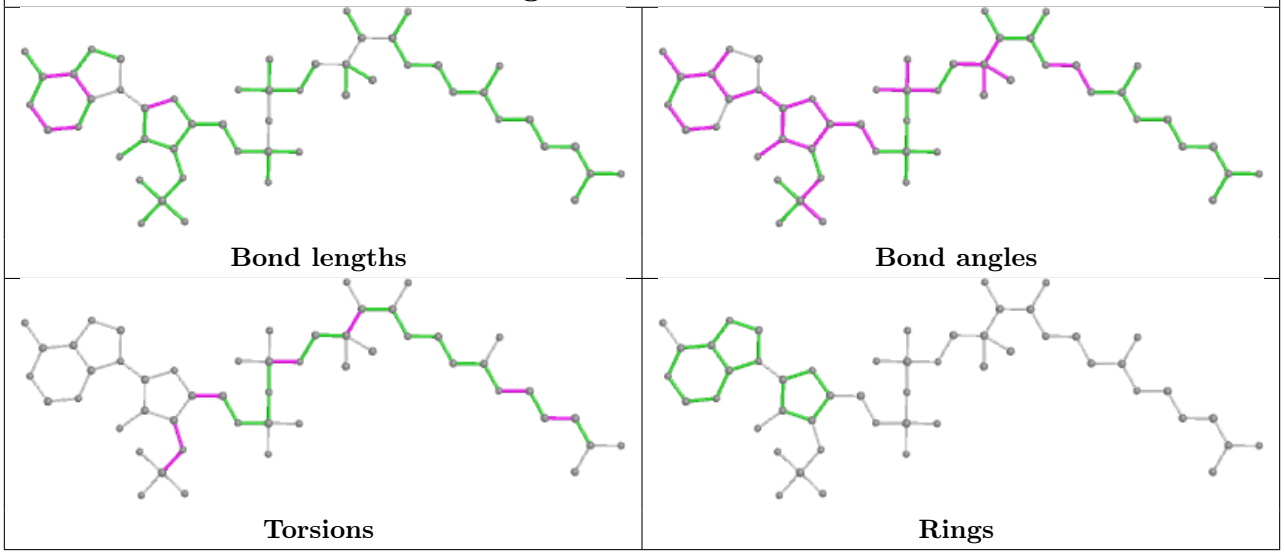
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



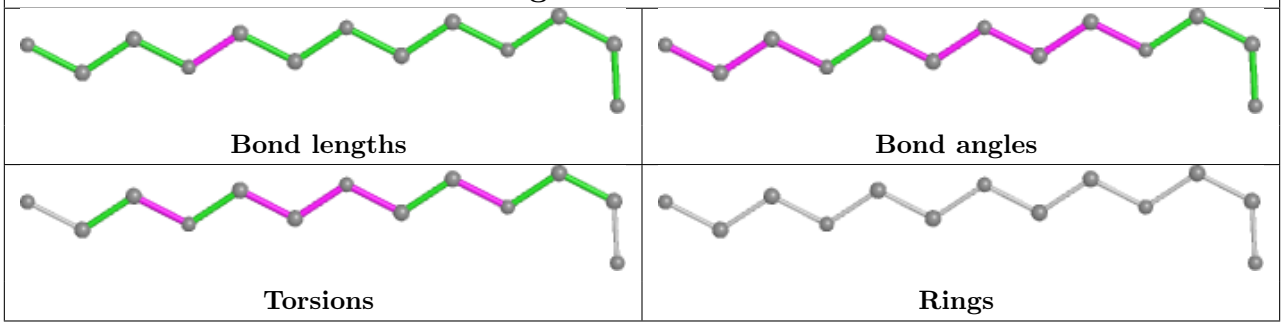
Ligand PE3 B 305



Ligand ACO A 301



Ligand PE3 B 304



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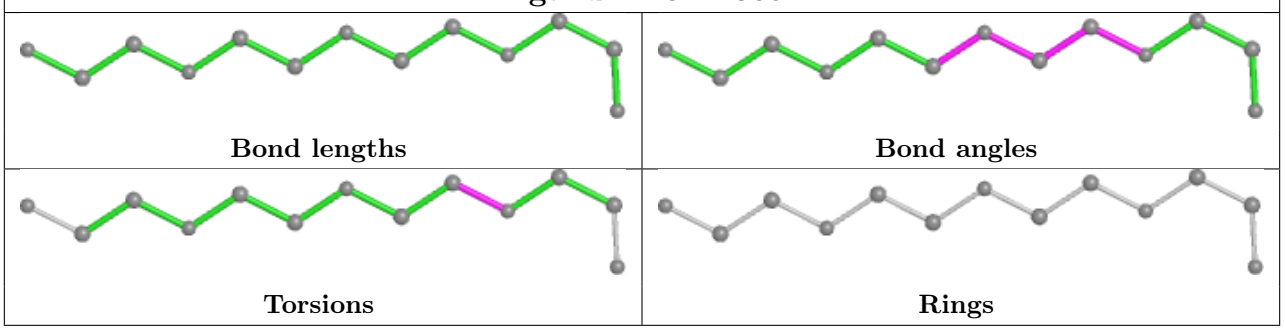
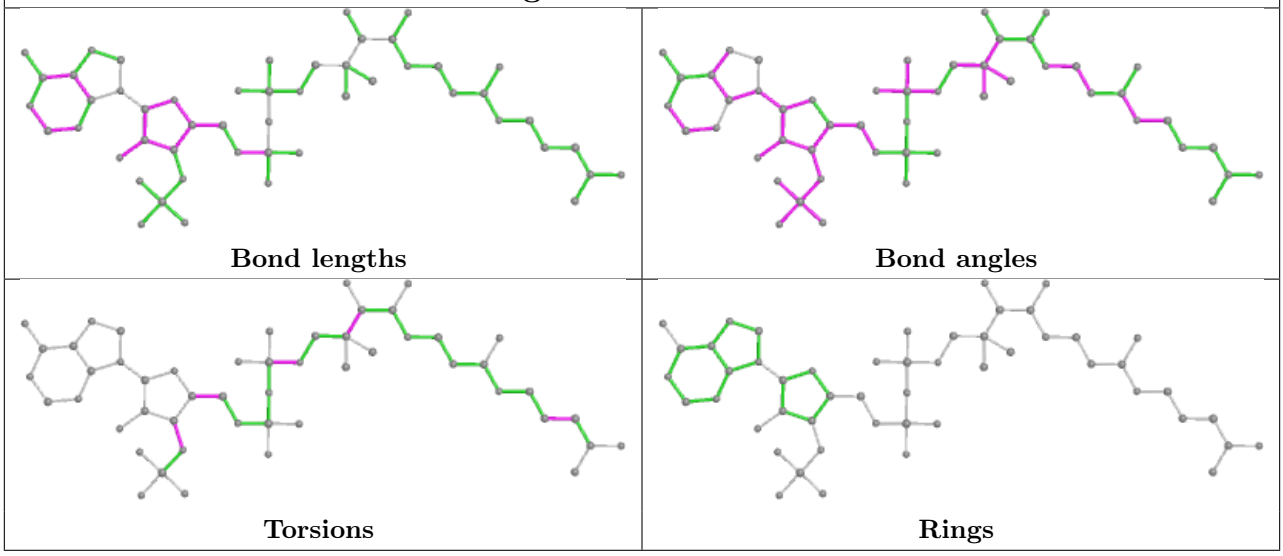
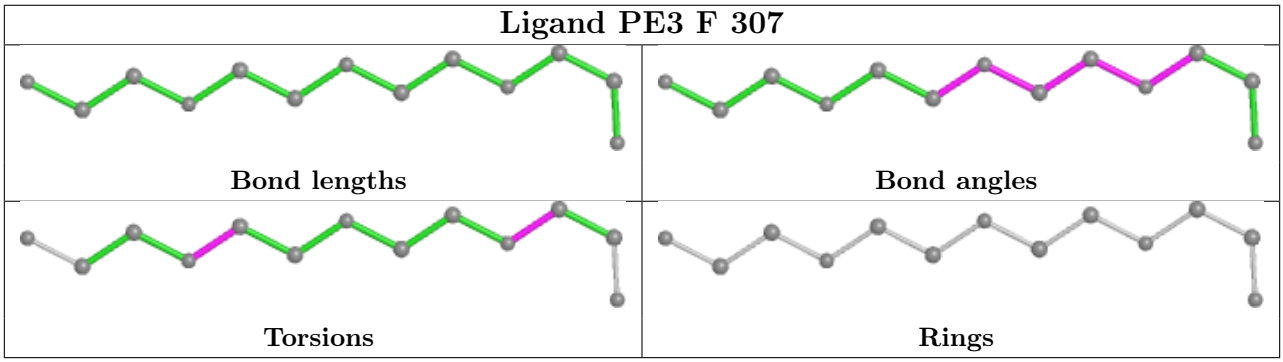


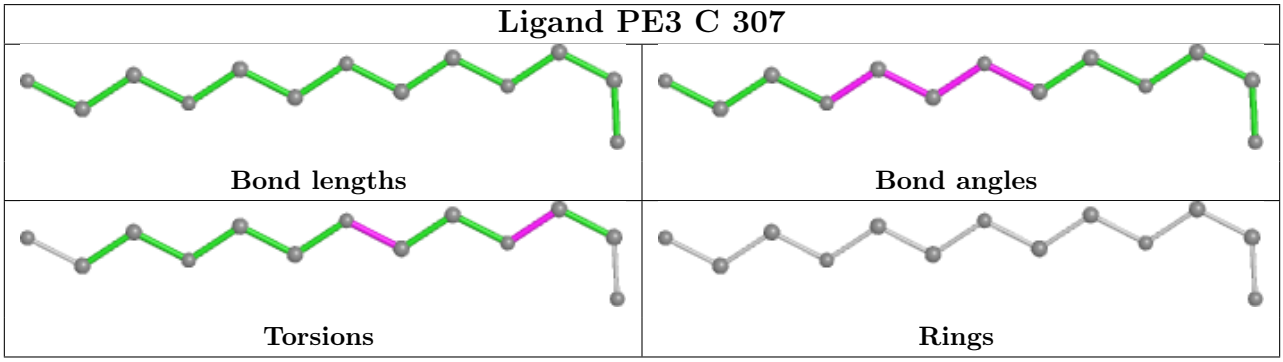
Ligand ACO B 301



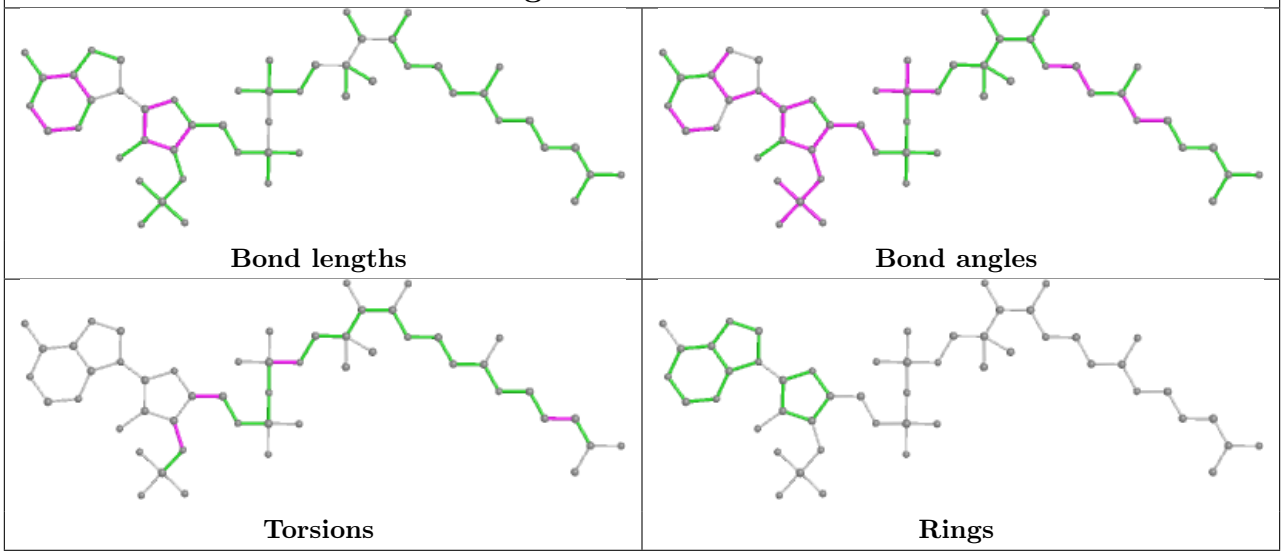
Ligand PE3 F 307



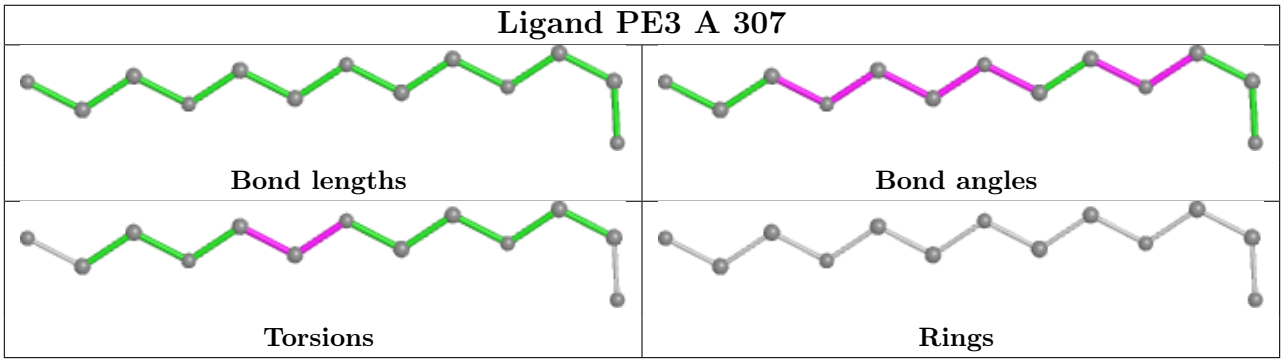
Ligand PE3 C 307



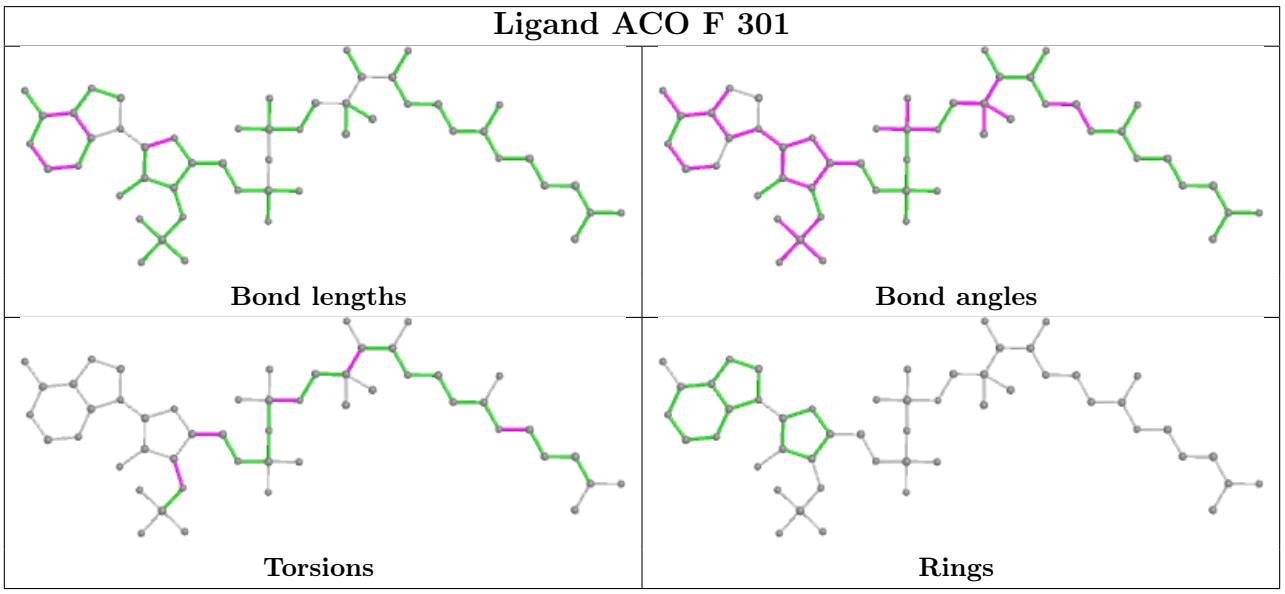
Ligand ACO E 301

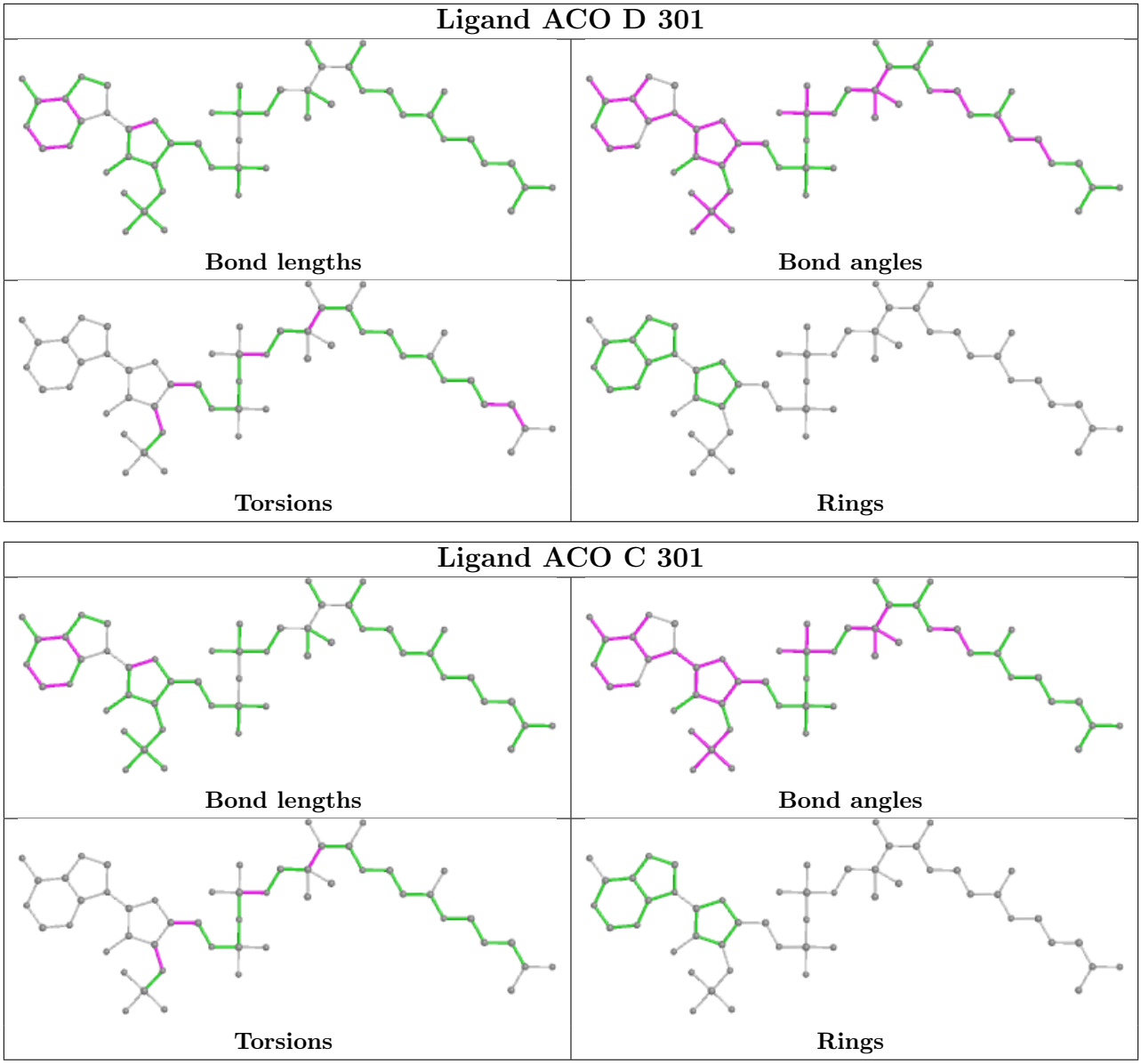


Ligand PE3 A 307



Ligand ACO F 301





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

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.