



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 10:37 AM EDT

PDB ID : 6N3P  
Title : Crosslinked AcpP=FabZ complex from E. coli Type II FAS  
Authors : Smith, J.L.; Dodge, G.J.  
Deposited on : 2018-11-15  
Resolution : 2.50 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)  
Xtrriage (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 2.50 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 4 unique types of molecules in this entry. The entry contains 10775 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 3-hydroxyacyl-[acyl-carrier-protein] dehydratase FabZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	144	1146	745	197	197	7	0	0	0
1	B	145	1153	749	198	199	7	0	0	0
1	C	144	1142	743	194	198	7	0	0	0
1	D	146	1161	753	200	201	7	0	0	0
1	E	146	1162	754	199	202	7	0	0	0
1	F	146	1162	754	199	202	7	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B7MBG1
A	-1	ASN	-	expression tag	UNP B7MBG1
A	0	ALA	-	expression tag	UNP B7MBG1
A	151	ALA	-	expression tag	UNP B7MBG1
B	-2	SER	-	expression tag	UNP B7MBG1
B	-1	ASN	-	expression tag	UNP B7MBG1
B	0	ALA	-	expression tag	UNP B7MBG1
B	151	ALA	-	expression tag	UNP B7MBG1
C	-2	SER	-	expression tag	UNP B7MBG1
C	-1	ASN	-	expression tag	UNP B7MBG1
C	0	ALA	-	expression tag	UNP B7MBG1
C	151	ALA	-	expression tag	UNP B7MBG1
D	-2	SER	-	expression tag	UNP B7MBG1
D	-1	ASN	-	expression tag	UNP B7MBG1
D	0	ALA	-	expression tag	UNP B7MBG1
D	151	ALA	-	expression tag	UNP B7MBG1
E	-2	SER	-	expression tag	UNP B7MBG1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP B7MBG1
E	0	ALA	-	expression tag	UNP B7MBG1
E	151	ALA	-	expression tag	UNP B7MBG1
F	-2	SER	-	expression tag	UNP B7MBG1
F	-1	ASN	-	expression tag	UNP B7MBG1
F	0	ALA	-	expression tag	UNP B7MBG1
F	151	ALA	-	expression tag	UNP B7MBG1

- Molecule 2 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	72	Total	C	N	O	S	0	0	0
			562	349	85	127	1			
2	H	75	Total	C	N	O	S	0	0	0
			585	362	91	131	1			
2	I	76	Total	C	N	O	S	0	0	0
			587	363	91	132	1			
2	J	73	Total	C	N	O	S	0	0	0
			566	351	86	128	1			
2	K	77	Total	C	N	O	S	0	0	0
			596	368	93	134	1			
2	L	70	Total	C	N	O	S	0	0	0
			547	341	82	123	1			

There are 18 discrepancies between the modelled and reference sequences:

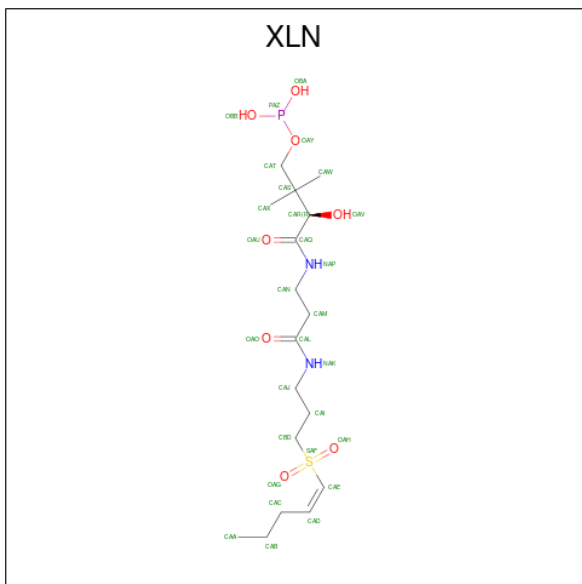
Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	SER	-	expression tag	UNP B7MJ81
G	-1	ASN	-	expression tag	UNP B7MJ81
G	0	ALA	-	expression tag	UNP B7MJ81
H	-2	SER	-	expression tag	UNP B7MJ81
H	-1	ASN	-	expression tag	UNP B7MJ81
H	0	ALA	-	expression tag	UNP B7MJ81
I	-2	SER	-	expression tag	UNP B7MJ81
I	-1	ASN	-	expression tag	UNP B7MJ81
I	0	ALA	-	expression tag	UNP B7MJ81
J	-2	SER	-	expression tag	UNP B7MJ81
J	-1	ASN	-	expression tag	UNP B7MJ81
J	0	ALA	-	expression tag	UNP B7MJ81
K	-2	SER	-	expression tag	UNP B7MJ81
K	-1	ASN	-	expression tag	UNP B7MJ81
K	0	ALA	-	expression tag	UNP B7MJ81

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP B7MJ81
L	-1	ASN	-	expression tag	UNP B7MJ81
L	0	ALA	-	expression tag	UNP B7MJ81

- Molecule 3 is N 3 -{(2R)-4-[(dihydroxyphosphanyl)oxy]-2-hydroxy-3,3-dimethylbutanoyl }-N-(3-[[1Z)-pent-1-en-1-yl]sulfonyl}propyl)-beta-alaninamide (three-letter code: XLN) (formula: C<sub>17</sub>H<sub>33</sub>N<sub>2</sub>O<sub>8</sub>PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	B	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	C	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	D	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	E	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		
3	F	1	Total	C	N	O	P	S	0	1
			58	34	4	16	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	5	Total 5	O 5	0	0
4	C	9	Total 9	O 9	0	0
4	D	6	Total 6	O 6	0	0
4	E	12	Total 12	O 12	0	0
4	F	5	Total 5	O 5	0	0
4	G	1	Total 1	O 1	0	0
4	H	1	Total 1	O 1	0	0
4	I	3	Total 3	O 3	0	0
4	J	4	Total 4	O 4	0	0
4	K	3	Total 3	O 3	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, $\alpha$ , $\beta$ , $\gamma$	65.14Å 136.19Å 152.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 2.50	Depositor
% Data completeness (in resolution range)	99.8 (49.49-2.50)	Depositor
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.37 (at 2.39Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.210 , 0.257	Depositor
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtrriage
Anisotropy	0.241	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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](#)

12 ligands are modelled in this entry.

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	XLN	A	400[B]	1,2	21,28,28	1.96	3 (14%)	27,37,37	3.35	2 (7%)
3	XLN	C	400[B]	1,2	21,28,28	2.13	3 (14%)	27,37,37	3.21	4 (14%)
3	XLN	F	400[A]	1,2	21,28,28	2.46	3 (14%)	27,37,37	3.96	1 (3%)
3	XLN	A	400[A]	1,2	21,28,28	3.31	8 (38%)	27,37,37	4.14	4 (14%)
3	XLN	C	400[A]	1,2	21,28,28	2.75	3 (14%)	27,37,37	3.85	5 (18%)
3	XLN	E	400[B]	1,2	21,28,28	3.62	7 (33%)	27,37,37	4.54	5 (18%)
3	XLN	B	400[B]	1,2	21,28,28	2.06	3 (14%)	27,37,37	3.62	1 (3%)
3	XLN	E	400[A]	1,2	21,28,28	1.88	2 (9%)	27,37,37	3.87	4 (14%)
3	XLN	B	400[A]	1,2	21,28,28	3.26	4 (19%)	27,37,37	4.28	6 (22%)
3	XLN	D	400[A]	1,2	21,28,28	2.42	3 (14%)	27,37,37	3.68	5 (18%)
3	XLN	D	400[B]	1,2	21,28,28	2.69	3 (14%)	27,37,37	3.78	7 (25%)
3	XLN	F	400[B]	1,2	21,28,28	2.57	3 (14%)	27,37,37	3.77	2 (7%)

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	XLN	A	400[B]	1,2	-	12/34/36/36	-
3	XLN	C	400[B]	1,2	-	14/34/36/36	-
3	XLN	F	400[A]	1,2	-	11/34/36/36	-
3	XLN	A	400[A]	1,2	-	16/34/36/36	-
3	XLN	C	400[A]	1,2	-	12/34/36/36	-
3	XLN	E	400[B]	1,2	-	18/34/36/36	-
3	XLN	B	400[B]	1,2	-	23/34/36/36	-
3	XLN	E	400[A]	1,2	-	16/34/36/36	-
3	XLN	B	400[A]	1,2	-	22/34/36/36	-
3	XLN	D	400[A]	1,2	-	13/34/36/36	-
3	XLN	D	400[B]	1,2	-	13/34/36/36	-
3	XLN	F	400[B]	1,2	-	10/34/36/36	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400[A]	XLN	CBD-SAF	-10.06	1.61	1.77
3	E	400[B]	XLN	CBD-SAF	-9.96	1.61	1.77
3	A	400[A]	XLN	CBD-SAF	-9.62	1.62	1.77
3	C	400[A]	XLN	CBD-SAF	-9.27	1.63	1.77
3	D	400[B]	XLN	CBD-SAF	-8.96	1.63	1.77
3	F	400[B]	XLN	CBD-SAF	-8.84	1.63	1.77
3	E	400[B]	XLN	OAH-SAF	-8.69	1.37	1.44
3	D	400[A]	XLN	CBD-SAF	-8.59	1.64	1.77
3	F	400[A]	XLN	CBD-SAF	-8.40	1.64	1.77
3	E	400[B]	XLN	OAG-SAF	-8.09	1.38	1.44
3	B	400[B]	XLN	CBD-SAF	-8.04	1.64	1.77
3	B	400[A]	XLN	OAH-SAF	-8.00	1.38	1.44
3	C	400[B]	XLN	CBD-SAF	-7.98	1.65	1.77
3	E	400[A]	XLN	CBD-SAF	-7.85	1.65	1.77
3	A	400[B]	XLN	CBD-SAF	-7.79	1.65	1.77
3	A	400[A]	XLN	OAH-SAF	-7.12	1.38	1.44
3	A	400[A]	XLN	OAG-SAF	-7.07	1.38	1.44
3	C	400[A]	XLN	OAG-SAF	-5.97	1.39	1.44
3	D	400[B]	XLN	OAG-SAF	-5.93	1.39	1.44
3	B	400[A]	XLN	OAG-SAF	-5.35	1.40	1.44
3	F	400[B]	XLN	OAH-SAF	-5.12	1.40	1.44
3	F	400[A]	XLN	OAH-SAF	-4.98	1.40	1.44
3	C	400[A]	XLN	OAH-SAF	-4.94	1.40	1.44
3	D	400[A]	XLN	OAG-SAF	-4.88	1.40	1.44
3	F	400[B]	XLN	OAG-SAF	-4.69	1.40	1.44
3	F	400[A]	XLN	OAG-SAF	-4.56	1.40	1.44
3	D	400[B]	XLN	OAH-SAF	-4.41	1.40	1.44
3	D	400[A]	XLN	OAH-SAF	-3.57	1.41	1.44
3	C	400[B]	XLN	OAH-SAF	-3.52	1.41	1.44
3	C	400[B]	XLN	OAG-SAF	-3.51	1.41	1.44
3	B	400[B]	XLN	OAH-SAF	-3.24	1.41	1.44
3	B	400[A]	XLN	OAQ-CAL	-2.89	1.17	1.23
3	B	400[B]	XLN	OAG-SAF	-2.61	1.42	1.44
3	E	400[B]	XLN	OAQ-CAQ	-2.58	1.18	1.23
3	A	400[A]	XLN	OAQ-CAL	-2.50	1.18	1.23
3	A	400[B]	XLN	OAG-SAF	-2.50	1.42	1.44
3	A	400[B]	XLN	OAH-SAF	-2.44	1.42	1.44
3	A	400[A]	XLN	OAQ-CAQ	-2.31	1.18	1.23
3	E	400[B]	XLN	OAQ-CAL	-2.20	1.18	1.23
3	A	400[A]	XLN	PAZ-OAY	-2.17	1.56	1.62
3	A	400[A]	XLN	CAW-CAS	-2.16	1.49	1.53
3	E	400[B]	XLN	CAQ-NAP	-2.15	1.29	1.33
3	E	400[A]	XLN	OAH-SAF	-2.07	1.42	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	400[B]	XLN	CAN-NAP	-2.02	1.41	1.46
3	A	400[A]	XLN	CAL-NAK	-2.02	1.28	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	400[B]	XLN	OAH-SAF-OAG	-21.84	106.32	118.22
3	B	400[A]	XLN	OAH-SAF-OAG	-20.73	106.93	118.22
3	A	400[A]	XLN	OAH-SAF-OAG	-20.50	107.05	118.22
3	F	400[A]	XLN	OAH-SAF-OAG	-20.21	107.21	118.22
3	E	400[A]	XLN	OAH-SAF-OAG	-19.01	107.86	118.22
3	F	400[B]	XLN	OAH-SAF-OAG	-18.95	107.89	118.22
3	C	400[A]	XLN	OAH-SAF-OAG	-18.72	108.02	118.22
3	D	400[B]	XLN	OAH-SAF-OAG	-18.15	108.33	118.22
3	B	400[B]	XLN	OAH-SAF-OAG	-18.12	108.35	118.22
3	D	400[A]	XLN	OAH-SAF-OAG	-17.80	108.52	118.22
3	A	400[B]	XLN	OAH-SAF-OAG	-16.84	109.05	118.22
3	C	400[B]	XLN	OAH-SAF-OAG	-15.57	109.74	118.22
3	E	400[B]	XLN	CAD-CAE-SAF	4.50	133.74	122.22
3	E	400[B]	XLN	OAH-SAF-CAE	4.30	114.94	108.86
3	D	400[A]	XLN	OAG-SAF-CAE	3.30	113.51	108.86
3	B	400[A]	XLN	CAW-CAS-CAR	-3.18	103.30	108.82
3	E	400[B]	XLN	CAW-CAS-CAR	-3.15	103.36	108.82
3	C	400[A]	XLN	CAN-CAM-CAL	-3.05	107.28	112.36
3	E	400[A]	XLN	OAH-SAF-CAE	3.02	113.13	108.86
3	A	400[A]	XLN	CAN-NAP-CAQ	-3.00	117.24	122.59
3	C	400[A]	XLN	CAN-NAP-CAQ	-2.96	117.31	122.59
3	D	400[B]	XLN	CAC-CAD-CAE	-2.94	120.16	125.51
3	B	400[A]	XLN	CAX-CAS-CAT	2.89	112.95	108.23
3	D	400[B]	XLN	OAG-SAF-CAE	2.81	112.82	108.86
3	B	400[A]	XLN	CAN-NAP-CAQ	-2.78	117.63	122.59
3	E	400[A]	XLN	CAW-CAS-CAT	2.78	112.77	108.23
3	C	400[A]	XLN	CAC-CAD-CAE	-2.76	120.48	125.51
3	F	400[B]	XLN	OAH-SAF-CAE	2.72	112.70	108.86
3	C	400[A]	XLN	CAJ-NAK-CAL	-2.68	117.86	122.84
3	C	400[B]	XLN	CAN-CAM-CAL	-2.65	107.94	112.36
3	D	400[A]	XLN	CAN-CAM-CAL	-2.63	107.97	112.36
3	D	400[B]	XLN	CAN-NAP-CAQ	-2.55	118.03	122.59
3	D	400[A]	XLN	CAN-NAP-CAQ	-2.49	118.15	122.59
3	E	400[A]	XLN	CAN-CAM-CAL	-2.47	108.24	112.36
3	B	400[A]	XLN	CAD-CAE-SAF	2.44	128.46	122.22
3	A	400[A]	XLN	CAW-CAS-CAR	-2.35	104.74	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	400[B]	XLN	CAJ-NAK-CAL	-2.28	118.60	122.84
3	A	400[B]	XLN	CAN-CAM-CAL	-2.27	108.58	112.36
3	D	400[B]	XLN	CAW-CAS-CAR	-2.12	105.14	108.82
3	C	400[B]	XLN	CAN-NAP-CAQ	-2.12	118.81	122.59
3	A	400[A]	XLN	CAD-CAE-SAF	2.12	127.64	122.22
3	D	400[A]	XLN	CAJ-NAK-CAL	-2.09	118.95	122.84
3	D	400[B]	XLN	CAN-CAM-CAL	-2.08	108.89	112.36
3	D	400[B]	XLN	CAJ-NAK-CAL	-2.05	119.03	122.84
3	B	400[A]	XLN	CAJ-NAK-CAL	-2.03	119.06	122.84
3	E	400[B]	XLN	CAN-CAM-CAL	-2.02	109.00	112.36

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400[A]	XLN	CAL-CAM-CAN-NAP
3	A	400[A]	XLN	NAP-CAQ-CAR-CAS
3	A	400[A]	XLN	NAP-CAQ-CAR-OAV
3	A	400[A]	XLN	OAU-CAQ-CAR-CAS
3	A	400[A]	XLN	OAU-CAQ-CAR-OAV
3	A	400[A]	XLN	CAR-CAQ-NAP-CAN
3	A	400[A]	XLN	CAI-CBD-SAF-OAG
3	A	400[A]	XLN	CAI-CBD-SAF-OAH
3	A	400[B]	XLN	CAL-CAM-CAN-NAP
3	A	400[B]	XLN	NAP-CAQ-CAR-CAS
3	A	400[B]	XLN	NAP-CAQ-CAR-OAV
3	A	400[B]	XLN	OAU-CAQ-CAR-CAS
3	A	400[B]	XLN	OAU-CAQ-CAR-OAV
3	A	400[B]	XLN	CAR-CAQ-NAP-CAN
3	A	400[B]	XLN	CAI-CBD-SAF-OAG
3	A	400[B]	XLN	CAI-CBD-SAF-OAH
3	B	400[A]	XLN	NAP-CAQ-CAR-CAS
3	B	400[A]	XLN	NAP-CAQ-CAR-OAV
3	B	400[A]	XLN	OAU-CAQ-CAR-CAS
3	B	400[A]	XLN	CAR-CAQ-NAP-CAN
3	B	400[A]	XLN	CAQ-CAR-CAS-CAT
3	B	400[A]	XLN	CAQ-CAR-CAS-CAW
3	B	400[A]	XLN	CAQ-CAR-CAS-CAX
3	B	400[A]	XLN	OAV-CAR-CAS-CAT
3	B	400[A]	XLN	OAV-CAR-CAS-CAW
3	B	400[A]	XLN	OAV-CAR-CAS-CAX
3	B	400[A]	XLN	CAR-CAS-CAT-OAY

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Mol	Chain	Res	Type	Atoms
3	B	400[A]	XLN	CAW-CAS-CAT-OAY
3	B	400[A]	XLN	CAX-CAS-CAT-OAY
3	B	400[A]	XLN	CAI-CBD-SAF-OAH
3	B	400[B]	XLN	CAD-CAE-SAF-CBD
3	B	400[B]	XLN	NAP-CAQ-CAR-CAS
3	B	400[B]	XLN	NAP-CAQ-CAR-OAV
3	B	400[B]	XLN	OAU-CAQ-CAR-CAS
3	B	400[B]	XLN	CAR-CAQ-NAP-CAN
3	B	400[B]	XLN	CAQ-CAR-CAS-CAT
3	B	400[B]	XLN	CAQ-CAR-CAS-CAW
3	B	400[B]	XLN	CAQ-CAR-CAS-CAX
3	B	400[B]	XLN	OAV-CAR-CAS-CAT
3	B	400[B]	XLN	OAV-CAR-CAS-CAW
3	B	400[B]	XLN	OAV-CAR-CAS-CAX
3	B	400[B]	XLN	CAR-CAS-CAT-OAY
3	B	400[B]	XLN	CAW-CAS-CAT-OAY
3	B	400[B]	XLN	CAX-CAS-CAT-OAY
3	B	400[B]	XLN	CAI-CBD-SAF-OAG
3	B	400[B]	XLN	CAI-CBD-SAF-OAH
3	C	400[A]	XLN	CAD-CAE-SAF-CBD
3	C	400[A]	XLN	CAD-CAE-SAF-OAG
3	C	400[A]	XLN	CAD-CAE-SAF-OAH
3	C	400[A]	XLN	CAJ-CAI-CBD-SAF
3	C	400[A]	XLN	CAL-CAM-CAN-NAP
3	C	400[A]	XLN	CAR-CAQ-NAP-CAN
3	C	400[A]	XLN	CAI-CBD-SAF-OAG
3	C	400[A]	XLN	CAI-CBD-SAF-OAH
3	C	400[B]	XLN	CAL-CAM-CAN-NAP
3	C	400[B]	XLN	CAR-CAQ-NAP-CAN
3	C	400[B]	XLN	CAI-CBD-SAF-OAG
3	C	400[B]	XLN	CAI-CBD-SAF-OAH
3	D	400[A]	XLN	CAL-CAM-CAN-NAP
3	D	400[A]	XLN	NAP-CAQ-CAR-CAS
3	D	400[A]	XLN	NAP-CAQ-CAR-OAV
3	D	400[A]	XLN	OAU-CAQ-CAR-CAS
3	D	400[A]	XLN	CAI-CBD-SAF-OAG
3	D	400[A]	XLN	CAI-CBD-SAF-OAH
3	D	400[B]	XLN	CAJ-CAI-CBD-SAF
3	D	400[B]	XLN	CAL-CAM-CAN-NAP
3	D	400[B]	XLN	NAP-CAQ-CAR-CAS
3	D	400[B]	XLN	NAP-CAQ-CAR-OAV
3	D	400[B]	XLN	OAU-CAQ-CAR-CAS

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Mol	Chain	Res	Type	Atoms
3	D	400[B]	XLN	CAI-CBD-SAF-OAG
3	D	400[B]	XLN	CAI-CBD-SAF-OAH
3	E	400[A]	XLN	CAR-CAQ-NAP-CAN
3	E	400[A]	XLN	CAQ-CAR-CAS-CAT
3	E	400[A]	XLN	CAQ-CAR-CAS-CAW
3	E	400[A]	XLN	CAQ-CAR-CAS-CAX
3	E	400[A]	XLN	OAV-CAR-CAS-CAT
3	E	400[A]	XLN	OAV-CAR-CAS-CAW
3	E	400[A]	XLN	OAV-CAR-CAS-CAX
3	E	400[A]	XLN	CAR-CAS-CAT-OAY
3	E	400[A]	XLN	CAW-CAS-CAT-OAY
3	E	400[A]	XLN	CAX-CAS-CAT-OAY
3	E	400[A]	XLN	CAI-CBD-SAF-OAG
3	E	400[A]	XLN	CAI-CBD-SAF-OAH
3	E	400[B]	XLN	CAD-CAE-SAF-CBD
3	E	400[B]	XLN	CAD-CAE-SAF-OAG
3	E	400[B]	XLN	CAD-CAE-SAF-OAH
3	E	400[B]	XLN	CBD-CAI-CAJ-NAK
3	E	400[B]	XLN	CAR-CAQ-NAP-CAN
3	E	400[B]	XLN	CAQ-CAR-CAS-CAT
3	E	400[B]	XLN	CAQ-CAR-CAS-CAW
3	E	400[B]	XLN	CAQ-CAR-CAS-CAX
3	E	400[B]	XLN	OAV-CAR-CAS-CAT
3	E	400[B]	XLN	OAV-CAR-CAS-CAW
3	E	400[B]	XLN	OAV-CAR-CAS-CAX
3	E	400[B]	XLN	CAR-CAS-CAT-OAY
3	E	400[B]	XLN	CAX-CAS-CAT-OAY
3	F	400[A]	XLN	CAD-CAE-SAF-CBD
3	F	400[A]	XLN	CAD-CAE-SAF-OAG
3	F	400[A]	XLN	CAD-CAE-SAF-OAH
3	F	400[A]	XLN	CAI-CBD-SAF-OAG
3	F	400[A]	XLN	CAI-CBD-SAF-OAH
3	F	400[B]	XLN	CAD-CAE-SAF-CBD
3	F	400[B]	XLN	CAI-CBD-SAF-OAH
3	E	400[A]	XLN	OAU-CAQ-NAP-CAN
3	A	400[A]	XLN	OAU-CAQ-NAP-CAN
3	A	400[B]	XLN	OAU-CAQ-NAP-CAN
3	B	400[B]	XLN	OAU-CAQ-NAP-CAN
3	C	400[A]	XLN	OAU-CAQ-NAP-CAN
3	E	400[B]	XLN	OAU-CAQ-NAP-CAN
3	B	400[A]	XLN	OAU-CAQ-NAP-CAN
3	A	400[A]	XLN	CBD-CAI-CAJ-NAK

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Mol	Chain	Res	Type	Atoms
3	D	400[B]	XLN	CBD-CAI-CAJ-NAK
3	F	400[B]	XLN	CBD-CAI-CAJ-NAK
3	C	400[B]	XLN	OAU-CAQ-NAP-CAN
3	E	400[B]	XLN	CAW-CAS-CAT-OAY
3	B	400[A]	XLN	CAJ-CAI-CBD-SAF
3	F	400[B]	XLN	CAJ-CAI-CBD-SAF
3	D	400[B]	XLN	CAR-CAQ-NAP-CAN
3	B	400[B]	XLN	CAA-CAB-CAC-CAD
3	C	400[B]	XLN	CAA-CAB-CAC-CAD
3	B	400[A]	XLN	CBD-CAI-CAJ-NAK
3	A	400[A]	XLN	OAO-CAL-NAK-CAJ
3	C	400[B]	XLN	OAU-CAQ-CAR-OAV
3	D	400[A]	XLN	OAU-CAQ-CAR-OAV
3	D	400[B]	XLN	OAU-CAQ-CAR-OAV
3	B	400[A]	XLN	OAO-CAL-NAK-CAJ
3	B	400[B]	XLN	OAO-CAL-NAK-CAJ
3	A	400[B]	XLN	CBD-CAI-CAJ-NAK
3	F	400[A]	XLN	CBD-CAI-CAJ-NAK
3	A	400[A]	XLN	CAM-CAL-NAK-CAJ
3	A	400[A]	XLN	CAJ-CAI-CBD-SAF
3	B	400[A]	XLN	CAM-CAL-NAK-CAJ
3	B	400[A]	XLN	CAI-CBD-SAF-OAG
3	E	400[B]	XLN	CAI-CBD-SAF-OAG
3	F	400[B]	XLN	CAI-CBD-SAF-OAG
3	D	400[B]	XLN	OAU-CAQ-NAP-CAN
3	B	400[B]	XLN	CAM-CAL-NAK-CAJ
3	C	400[B]	XLN	NAP-CAQ-CAR-OAV
3	F	400[B]	XLN	CAB-CAC-CAD-CAE
3	D	400[A]	XLN	CAJ-CAI-CBD-SAF
3	F	400[A]	XLN	CAJ-CAI-CBD-SAF
3	D	400[A]	XLN	CAR-CAQ-NAP-CAN
3	D	400[A]	XLN	CAI-CAJ-NAK-CAL
3	A	400[A]	XLN	CAI-CBD-SAF-CAE
3	C	400[B]	XLN	CAI-CBD-SAF-CAE
3	D	400[B]	XLN	CAI-CBD-SAF-CAE
3	E	400[A]	XLN	CAI-CBD-SAF-CAE
3	F	400[B]	XLN	CAD-CAE-SAF-OAG
3	C	400[A]	XLN	OAU-CAQ-CAR-OAV
3	C	400[B]	XLN	CAX-CAS-CAT-OAY
3	B	400[B]	XLN	CBD-CAI-CAJ-NAK
3	D	400[A]	XLN	OAU-CAQ-NAP-CAN
3	B	400[B]	XLN	CAJ-CAI-CBD-SAF

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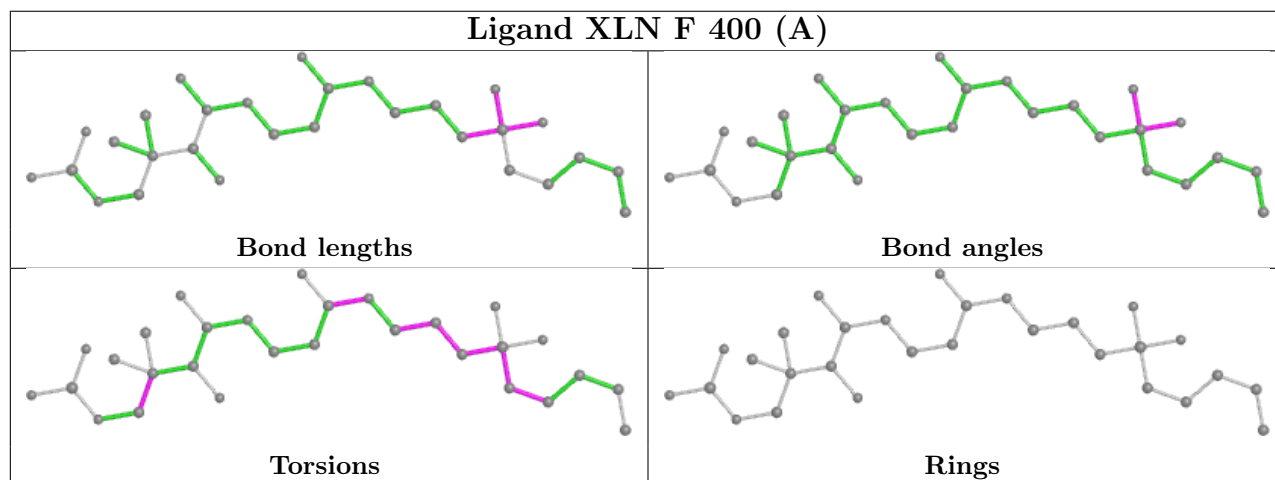
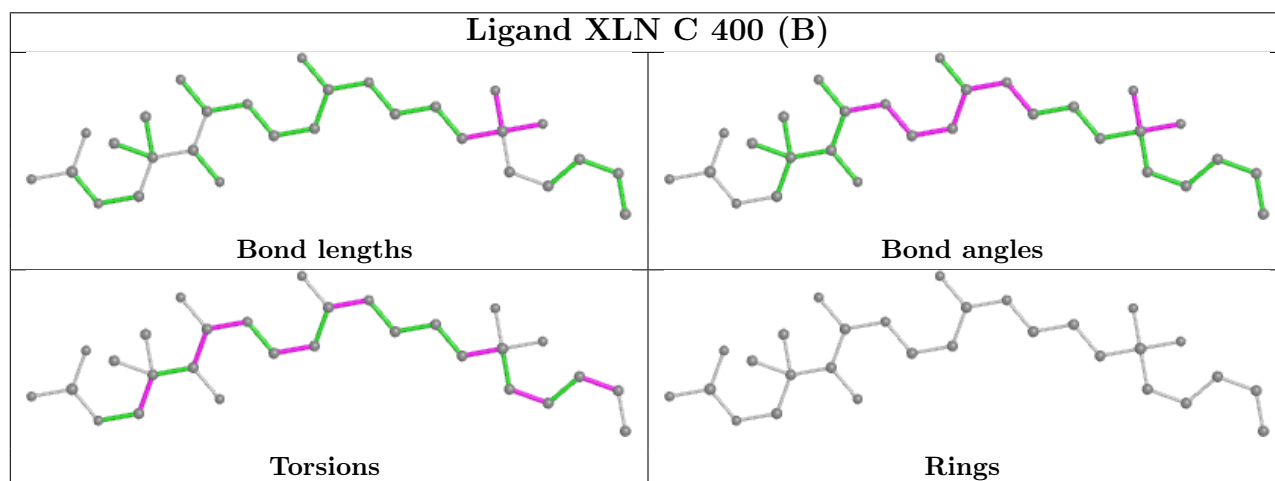
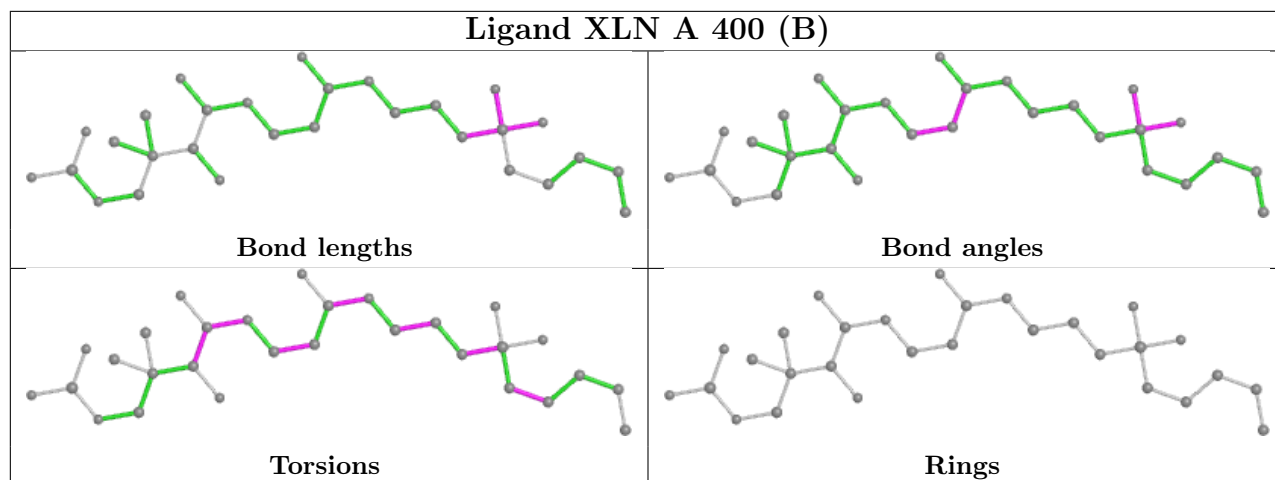
Mol	Chain	Res	Type	Atoms
3	B	400[A]	XLN	CAB-CAC-CAD-CAE
3	D	400[A]	XLN	CAA-CAB-CAC-CAD
3	E	400[B]	XLN	CAI-CBD-SAF-OAH
3	C	400[A]	XLN	CAX-CAS-CAT-OAY
3	F	400[A]	XLN	CAW-CAS-CAT-OAY
3	F	400[B]	XLN	CAW-CAS-CAT-OAY
3	F	400[A]	XLN	OAO-CAL-NAK-CAJ
3	C	400[B]	XLN	NAP-CAQ-CAR-CAS
3	A	400[A]	XLN	CAC-CAD-CAE-SAF
3	A	400[B]	XLN	CAC-CAD-CAE-SAF
3	B	400[A]	XLN	CAC-CAD-CAE-SAF
3	B	400[B]	XLN	CAC-CAD-CAE-SAF
3	C	400[A]	XLN	CAC-CAD-CAE-SAF
3	C	400[B]	XLN	CAC-CAD-CAE-SAF
3	D	400[A]	XLN	CAC-CAD-CAE-SAF
3	D	400[B]	XLN	CAC-CAD-CAE-SAF
3	E	400[A]	XLN	CAC-CAD-CAE-SAF
3	E	400[B]	XLN	CAC-CAD-CAE-SAF
3	F	400[A]	XLN	CAC-CAD-CAE-SAF
3	F	400[B]	XLN	CAC-CAD-CAE-SAF
3	A	400[B]	XLN	OAO-CAL-NAK-CAJ
3	E	400[A]	XLN	CAB-CAC-CAD-CAE
3	F	400[A]	XLN	CAX-CAS-CAT-OAY
3	C	400[B]	XLN	OAO-CAL-NAK-CAJ
3	A	400[A]	XLN	CAD-CAE-SAF-CBD
3	F	400[B]	XLN	OAO-CAL-NAK-CAJ
3	C	400[B]	XLN	OAU-CAQ-CAR-CAS

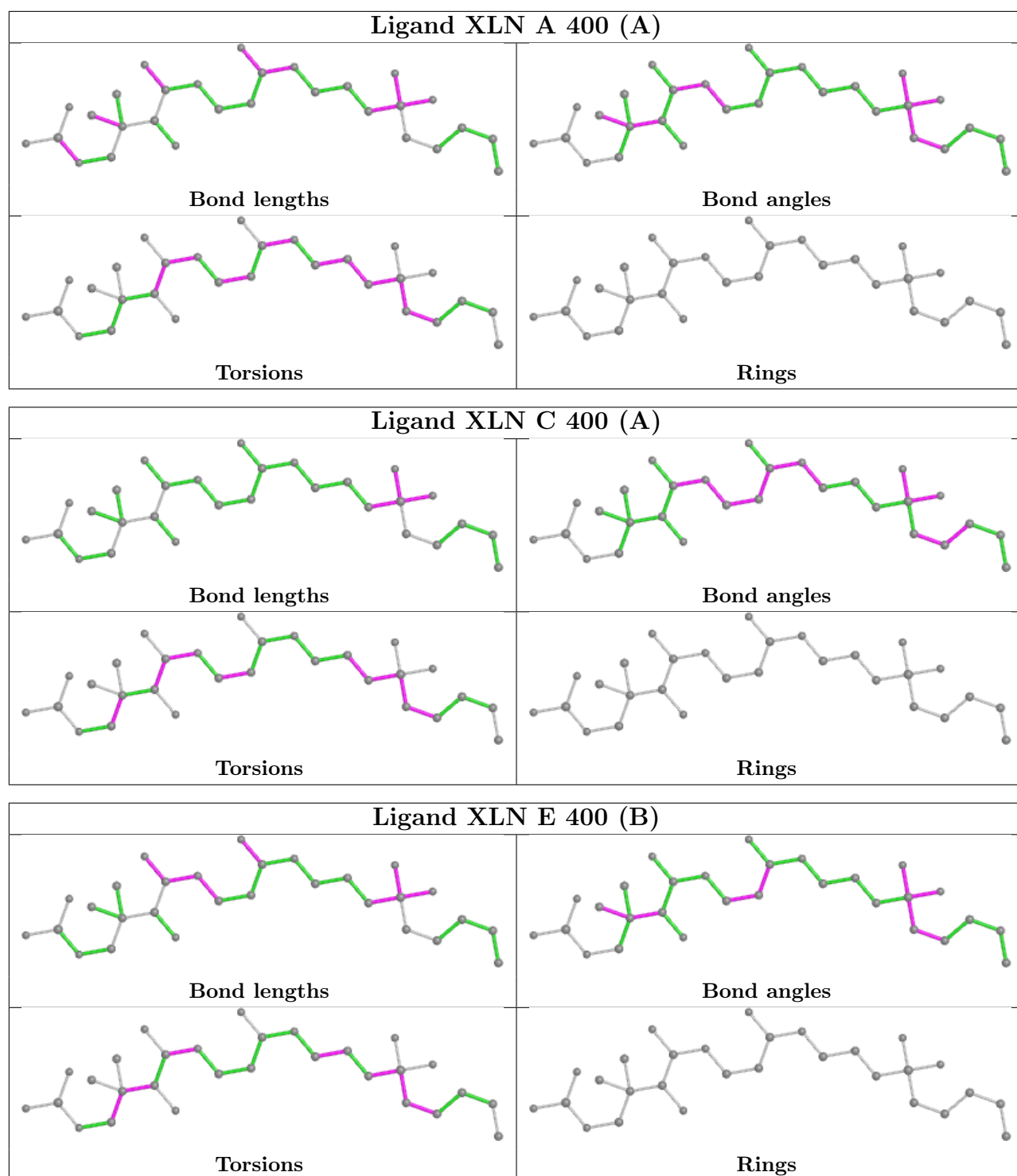
There are no ring outliers.

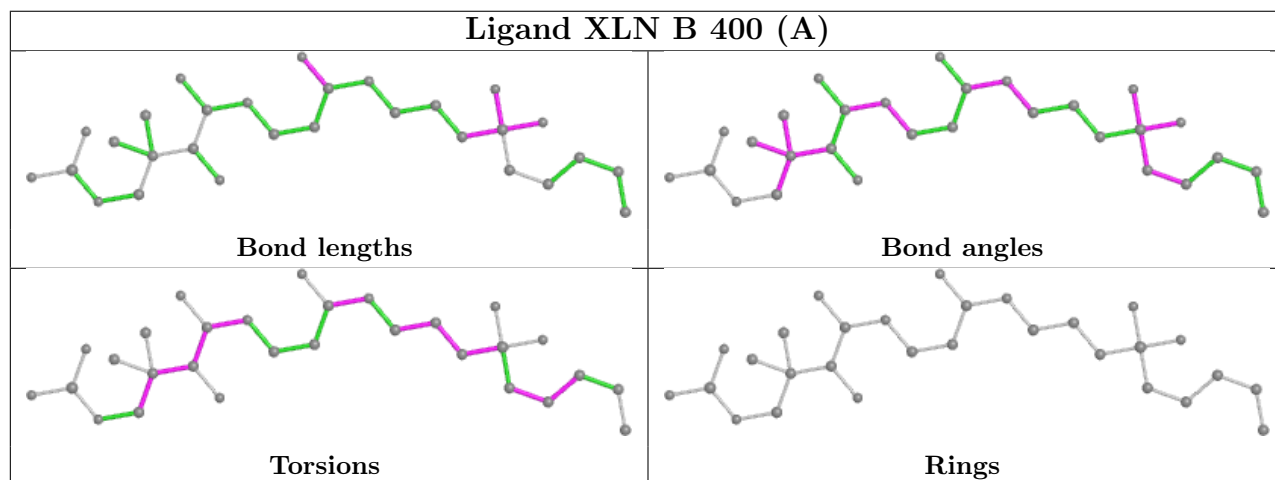
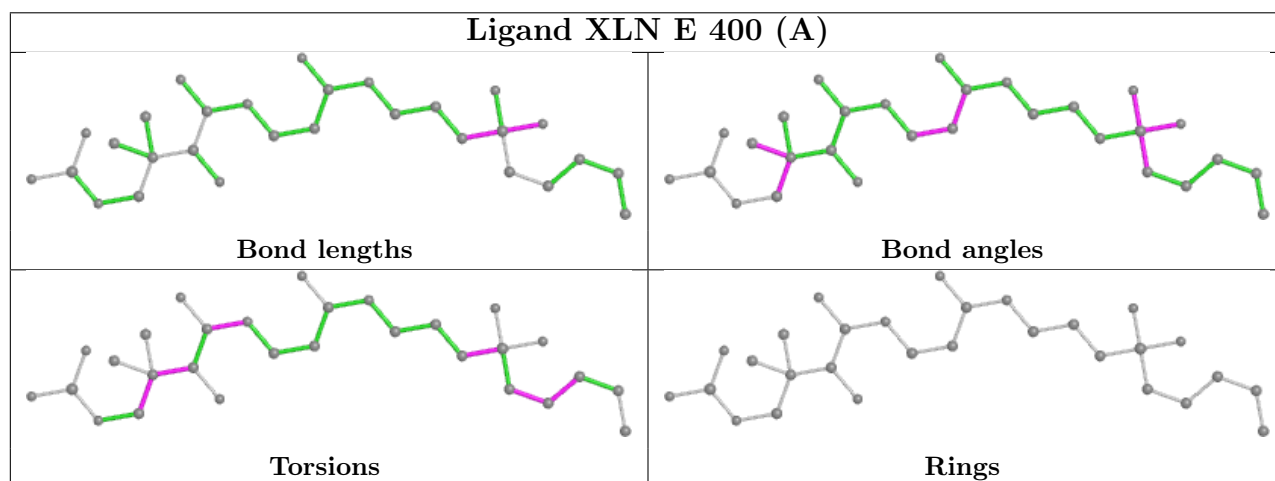
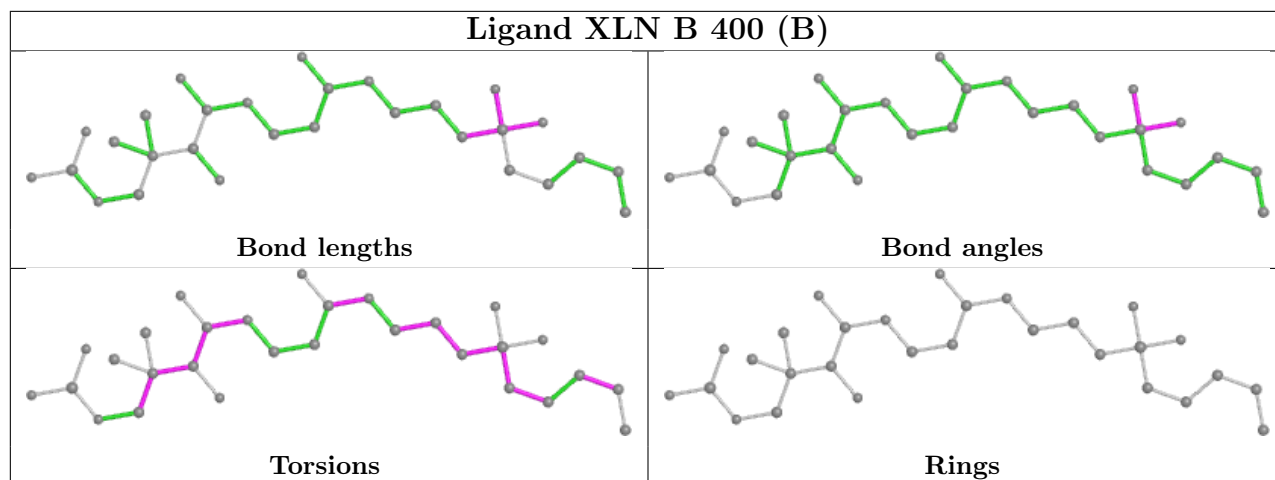
No monomer is involved in short contacts.

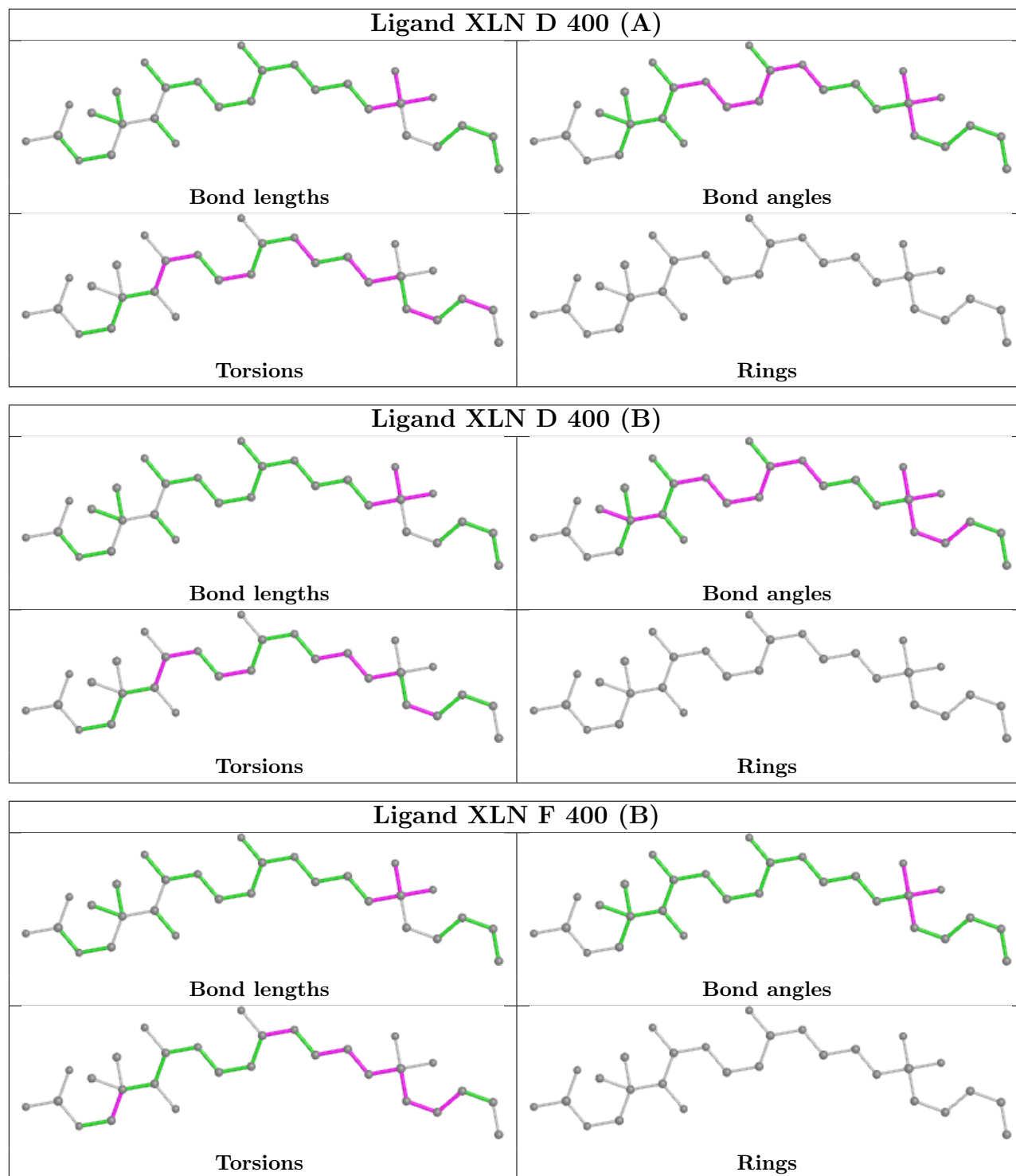
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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