



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 08:10 PM EDT

PDB ID : 6U49  
Title : Structure-based discovery of a novel small-molecule inhibitor of methicillin-resistant *S. aureus*  
Authors : Liu, J.; Kozhaya, L.; Torres, V.J.; Unutmaz, D.; Lu, M.  
Deposited on : 2019-08-23  
Resolution : 2.35 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 2.35 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](#)

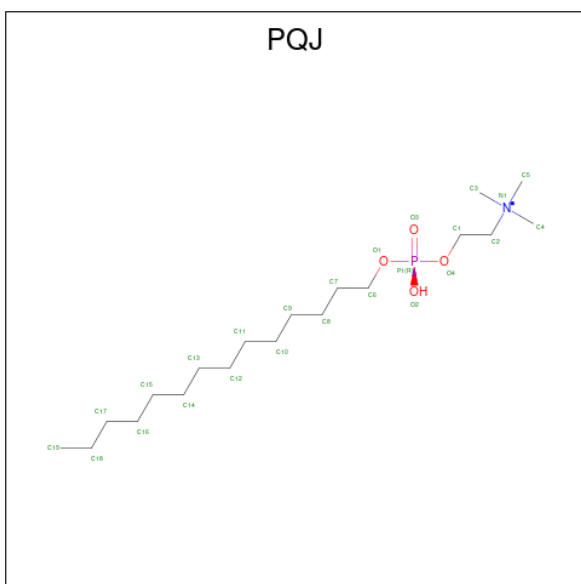
There are 4 unique types of molecules in this entry. The entry contains 17541 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	Total 2345	C 1472	N 401	O 465	S 7	0	0	0
1	B	293	Total 2345	C 1472	N 401	O 465	S 7	0	0	0
1	C	293	Total 2345	C 1472	N 401	O 465	S 7	0	0	0
1	D	293	Total 2345	C 1472	N 401	O 465	S 7	0	0	0
1	E	293	Total 2345	C 1472	N 401	O 465	S 7	0	0	0
1	F	293	Total 2345	C 1472	N 401	O 465	S 7	0	0	0
1	G	293	Total 2345	C 1472	N 401	O 465	S 7	0	0	0

- Molecule 2 is fos-choline-14 (three-letter code: PQJ) (formula:  $C_{19}H_{43}NO_4P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	B	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	D	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	D	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	F	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	F	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
2	G	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	P	0	0
			12	6	1	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		
4	B	133	Total	O	0	0
			133	133		
4	C	95	Total	O	0	0
			95	95		
4	D	114	Total	O	0	0
			114	114		
4	E	123	Total	O	0	0
			123	123		
4	F	141	Total	O	0	0
			141	141		
4	G	130	Total	O	0	0
			130	130		

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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.37Å 135.04Å 132.45Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	132.40 – 2.35	Depositor
% Data completeness (in resolution range)	94.3 (132.40-2.35)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.194 , 0.239	Depositor
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtrriage
Anisotropy	0.616	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtrriage
Total number of atoms	17541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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](#)

26 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	SO4	E	405	-	4,4,4	0.55	0	6,6,6	0.48	0
2	PQJ	D	402	-	11,11,24	0.87	0	15,16,29	0.87	1 (6%)
3	SO4	C	403	-	4,4,4	0.80	0	6,6,6	0.42	0
3	SO4	G	403	-	4,4,4	0.72	0	6,6,6	0.37	0
2	PQJ	F	304	-	10,10,24	0.98	1 (10%)	15,15,29	1.26	2 (13%)
2	PQJ	C	401	-	11,11,24	0.81	0	15,16,29	0.87	1 (6%)
3	SO4	D	404	-	4,4,4	0.83	0	6,6,6	0.38	0
2	PQJ	F	301	-	11,11,24	0.77	0	15,16,29	0.88	0
2	PQJ	E	401	-	11,11,24	0.86	0	15,16,29	0.92	0
2	PQJ	F	302	-	11,11,24	0.90	1 (9%)	15,16,29	1.31	2 (13%)
2	PQJ	G	401	-	11,11,24	0.84	0	15,16,29	0.78	1 (6%)
2	PQJ	G	402	-	11,11,24	0.96	0	15,16,29	1.05	1 (6%)
2	PQJ	B	401	-	10,10,24	0.99	0	15,15,29	1.37	3 (20%)
2	PQJ	B	402	-	11,11,24	0.78	0	15,16,29	0.91	1 (6%)
2	PQJ	C	402	-	10,10,24	1.00	1 (10%)	15,15,29	1.00	0
3	SO4	B	404	-	4,4,4	0.44	0	6,6,6	0.14	0
2	PQJ	A	403	-	10,10,24	1.41	1 (10%)	15,15,29	1.19	2 (13%)
2	PQJ	D	403	-	11,11,24	1.05	1 (9%)	15,16,29	1.05	1 (6%)
2	PQJ	E	404	-	10,10,24	1.41	1 (10%)	15,15,29	1.36	3 (20%)
2	PQJ	A	401	-	11,11,24	0.82	0	15,16,29	0.94	1 (6%)
2	PQJ	A	402	-	11,11,24	0.94	1 (9%)	15,16,29	0.85	0
2	PQJ	E	403	-	10,10,24	1.06	1 (10%)	15,15,29	0.87	1 (6%)
2	PQJ	F	303	-	10,10,24	1.02	1 (10%)	15,15,29	1.01	2 (13%)
2	PQJ	E	402	-	11,11,24	1.01	1 (9%)	15,16,29	0.82	0
2	PQJ	D	401	-	10,10,24	1.46	1 (10%)	15,15,29	1.28	1 (6%)
2	PQJ	B	403	-	11,11,24	0.69	0	15,16,29	1.06	0

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	PQJ	D	402	-	-	4/11/11/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PQJ	F	304	-	-	3/8/8/24	-
2	PQJ	C	401	-	-	7/11/11/24	-
2	PQJ	F	301	-	-	5/11/11/24	-
2	PQJ	E	401	-	-	3/11/11/24	-
2	PQJ	F	302	-	-	4/11/11/24	-
2	PQJ	G	401	-	-	2/11/11/24	-
2	PQJ	G	402	-	-	4/11/11/24	-
2	PQJ	B	401	-	-	3/8/8/24	-
2	PQJ	B	402	-	-	1/11/11/24	-
2	PQJ	C	402	-	-	4/8/8/24	-
2	PQJ	A	403	-	-	2/8/8/24	-
2	PQJ	D	403	-	-	4/11/11/24	-
2	PQJ	E	404	-	-	3/8/8/24	-
2	PQJ	A	401	-	-	5/11/11/24	-
2	PQJ	A	402	-	-	7/11/11/24	-
2	PQJ	E	403	-	-	3/8/8/24	-
2	PQJ	F	303	-	-	3/8/8/24	-
2	PQJ	E	402	-	-	3/11/11/24	-
2	PQJ	D	401	-	-	3/8/8/24	-
2	PQJ	B	403	-	-	4/11/11/24	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	403	PQJ	P1-O3	3.95	1.63	1.50
2	E	404	PQJ	P1-O3	3.94	1.63	1.50
2	D	401	PQJ	P1-O3	3.89	1.63	1.50
2	D	403	PQJ	P1-O1	2.45	1.68	1.59
2	F	304	PQJ	P1-O1	2.44	1.64	1.54
2	E	403	PQJ	P1-O1	2.31	1.63	1.54
2	F	303	PQJ	P1-O1	2.30	1.63	1.54
2	F	302	PQJ	P1-O1	2.24	1.67	1.59
2	C	402	PQJ	P1-O1	2.12	1.63	1.54
2	E	402	PQJ	P1-O1	2.06	1.66	1.59
2	A	402	PQJ	P1-O1	2.01	1.66	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PQJ	O1-P1-O2	4.04	123.07	107.64
2	E	404	PQJ	O1-P1-O2	3.22	119.93	107.64
2	F	302	PQJ	O2-P1-O1	2.91	118.36	105.88
2	A	403	PQJ	O4-P1-O3	-2.88	98.40	106.47
2	A	403	PQJ	O1-P1-O2	2.79	118.30	107.64
2	B	401	PQJ	O1-P1-O4	-2.70	99.56	106.73
2	F	304	PQJ	O2-P1-O3	2.65	121.04	110.68
2	B	401	PQJ	P1-O4-C1	2.53	125.25	118.30
2	D	403	PQJ	C3-N1-C4	-2.39	102.84	108.97
2	A	401	PQJ	O2-P1-O1	2.36	115.98	105.88
2	B	402	PQJ	C3-N1-C5	-2.34	102.96	108.97
2	F	304	PQJ	C3-N1-C4	-2.30	103.06	108.97
2	C	401	PQJ	C3-N1-C5	-2.27	103.13	108.97
2	G	402	PQJ	O2-P1-O1	2.24	115.48	105.88
2	E	404	PQJ	C3-N1-C4	-2.23	103.25	108.97
2	F	303	PQJ	O2-P1-O3	2.19	119.27	110.68
2	G	401	PQJ	O2-P1-O3	2.14	122.80	112.24
2	B	401	PQJ	O2-P1-O3	2.09	118.87	110.68
2	E	404	PQJ	C4-N1-C2	2.04	118.28	109.92
2	F	302	PQJ	O2-P1-O4	-2.03	98.32	107.75
2	E	403	PQJ	O2-P1-O3	2.03	118.62	110.68
2	F	303	PQJ	O1-P1-O4	-2.01	101.38	106.73
2	D	402	PQJ	O4-P1-O3	-2.00	101.25	109.07

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	PQJ	C1-O4-P1-O2
2	A	402	PQJ	C1-O4-P1-O3
2	A	402	PQJ	C1-O4-P1-O1
2	A	402	PQJ	C6-O1-P1-O2
2	B	402	PQJ	O4-C1-C2-N1
2	B	403	PQJ	C1-O4-P1-O3
2	C	402	PQJ	C1-O4-P1-O2
2	C	402	PQJ	C1-O4-P1-O3
2	C	402	PQJ	C1-O4-P1-O1
2	C	402	PQJ	O4-C1-C2-N1
2	D	403	PQJ	C6-O1-P1-O2
2	D	403	PQJ	C6-O1-P1-O3
2	D	403	PQJ	C6-O1-P1-O4
2	E	401	PQJ	C1-O4-P1-O3
2	F	302	PQJ	C1-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
2	F	302	PQJ	C6-O1-P1-O3
2	G	401	PQJ	C1-O4-P1-O2
2	G	402	PQJ	C1-C2-N1-C4
2	D	402	PQJ	C1-C2-N1-C4
2	G	402	PQJ	C1-C2-N1-C5
2	E	404	PQJ	C1-C2-N1-C5
2	E	404	PQJ	C1-C2-N1-C4
2	E	402	PQJ	C1-O4-P1-O1
2	D	402	PQJ	C1-C2-N1-C3
2	C	401	PQJ	C6-O1-P1-O3
2	F	301	PQJ	C6-O1-P1-O3
2	D	402	PQJ	C1-C2-N1-C5
2	E	404	PQJ	C1-C2-N1-C3
2	G	402	PQJ	C1-C2-N1-C3
2	B	401	PQJ	C1-C2-N1-C5
2	C	401	PQJ	C1-C2-N1-C5
2	A	403	PQJ	C1-O4-P1-O3
2	F	304	PQJ	C1-C2-N1-C3
2	A	402	PQJ	C6-O1-P1-O3
2	D	401	PQJ	C1-C2-N1-C5
2	A	401	PQJ	C6-O1-P1-O3
2	E	401	PQJ	C1-O4-P1-O1
2	E	401	PQJ	C1-O4-P1-O2
2	E	402	PQJ	C1-O4-P1-O2
2	E	402	PQJ	C1-O4-P1-O3
2	F	301	PQJ	C1-C2-N1-C3
2	B	401	PQJ	C1-C2-N1-C4
2	C	401	PQJ	C1-C2-N1-C4
2	D	401	PQJ	C1-C2-N1-C4
2	F	301	PQJ	C1-C2-N1-C4
2	F	304	PQJ	C1-C2-N1-C4
2	B	401	PQJ	C1-C2-N1-C3
2	C	401	PQJ	C6-O1-P1-O4
2	D	401	PQJ	C1-C2-N1-C3
2	E	403	PQJ	C1-C2-N1-C3
2	B	403	PQJ	C1-O4-P1-O1
2	F	304	PQJ	C1-C2-N1-C5
2	B	403	PQJ	C6-O1-P1-O2
2	C	401	PQJ	C6-O1-P1-O2
2	D	402	PQJ	C6-O1-P1-O2
2	F	301	PQJ	C6-O1-P1-O2
2	A	401	PQJ	C1-C2-N1-C5

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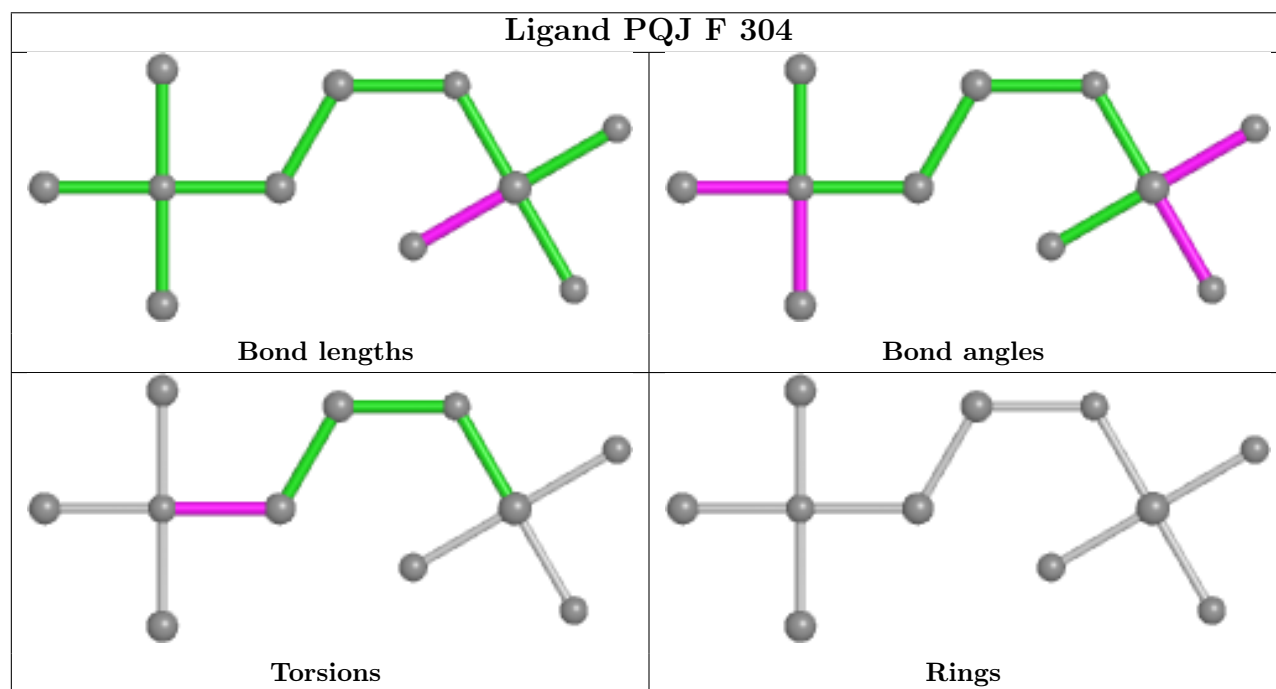
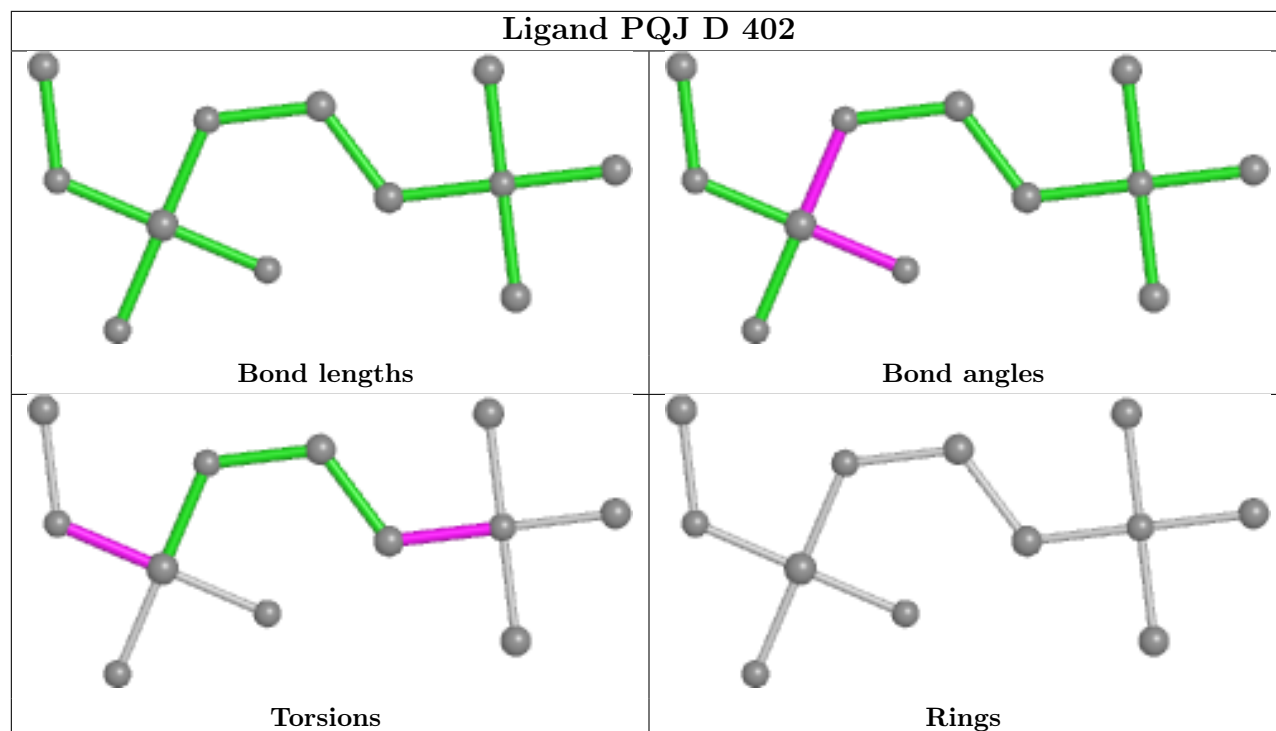
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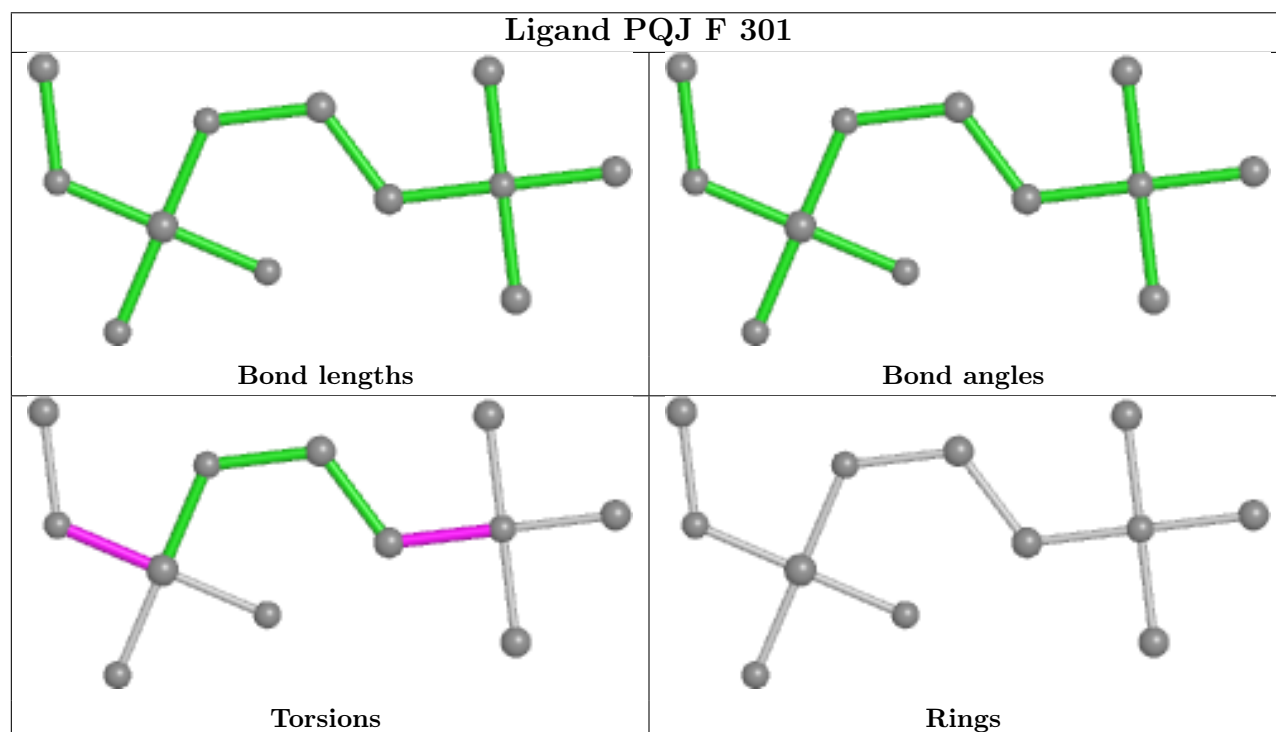
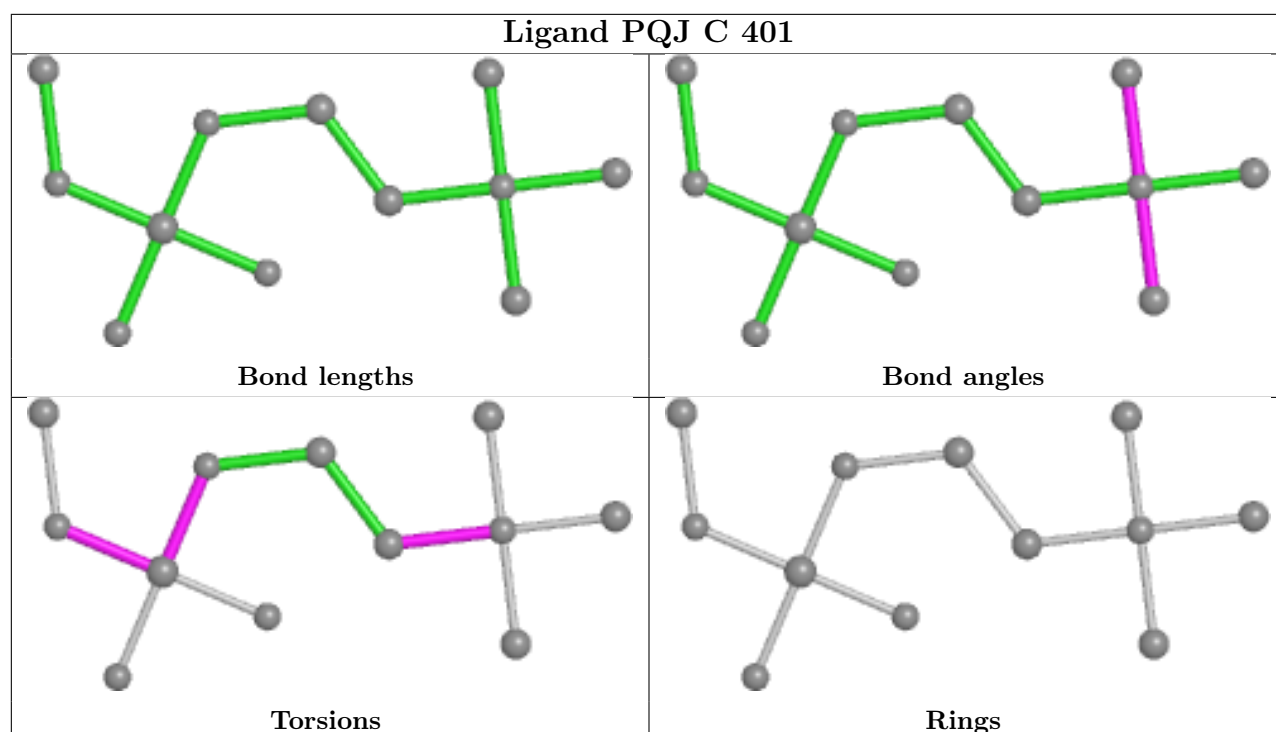
Mol	Chain	Res	Type	Atoms
2	C	401	PQJ	C1-C2-N1-C3
2	F	301	PQJ	C1-C2-N1-C5
2	F	303	PQJ	C1-C2-N1-C3
2	A	402	PQJ	C1-C2-N1-C5
2	E	403	PQJ	C1-C2-N1-C4
2	F	302	PQJ	C1-O4-P1-O1
2	A	401	PQJ	C1-C2-N1-C3
2	E	403	PQJ	C1-C2-N1-C5
2	A	402	PQJ	C1-C2-N1-C4
2	F	303	PQJ	C1-C2-N1-C4
2	F	302	PQJ	C1-C2-N1-C5
2	A	401	PQJ	C6-O1-P1-O4
2	A	401	PQJ	C1-C2-N1-C4
2	A	403	PQJ	C1-C2-N1-C4
2	C	401	PQJ	C1-O4-P1-O3
2	D	403	PQJ	C1-O4-P1-O3
2	G	401	PQJ	C1-O4-P1-O3
2	G	402	PQJ	C1-O4-P1-O2
2	B	403	PQJ	C1-C2-N1-C3
2	F	303	PQJ	C1-C2-N1-C5

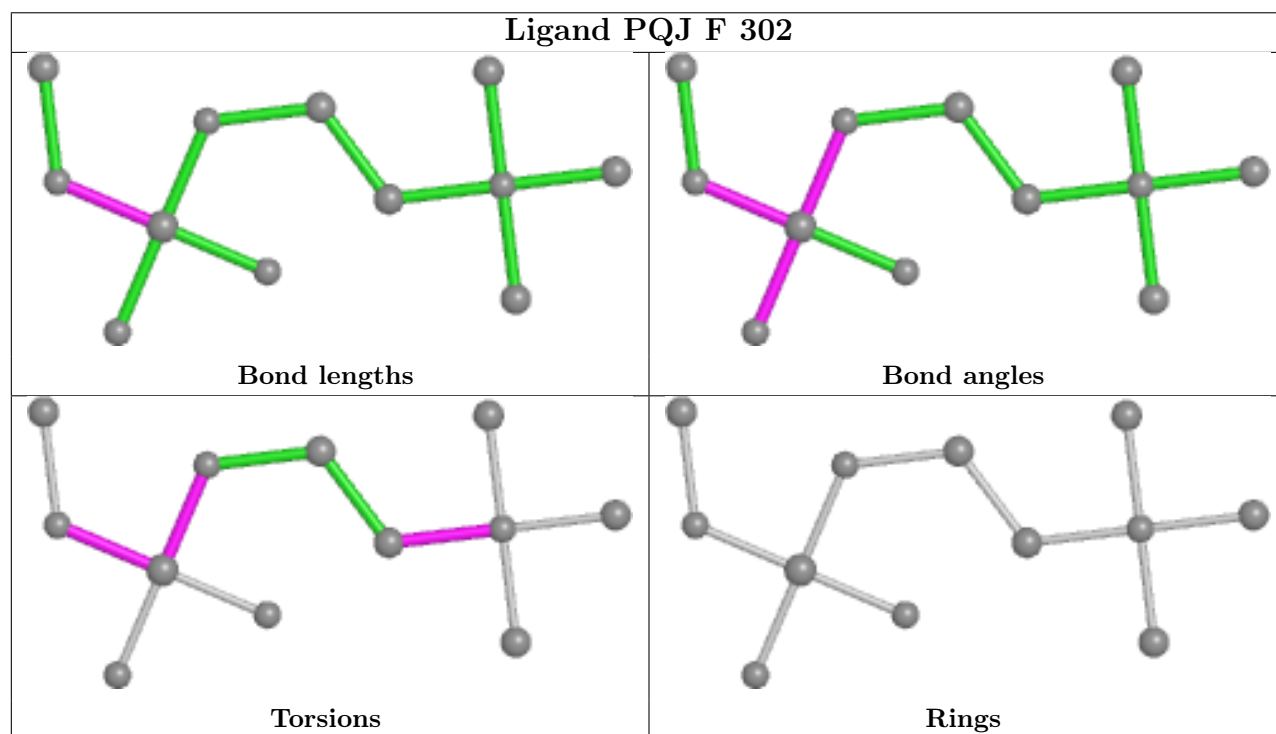
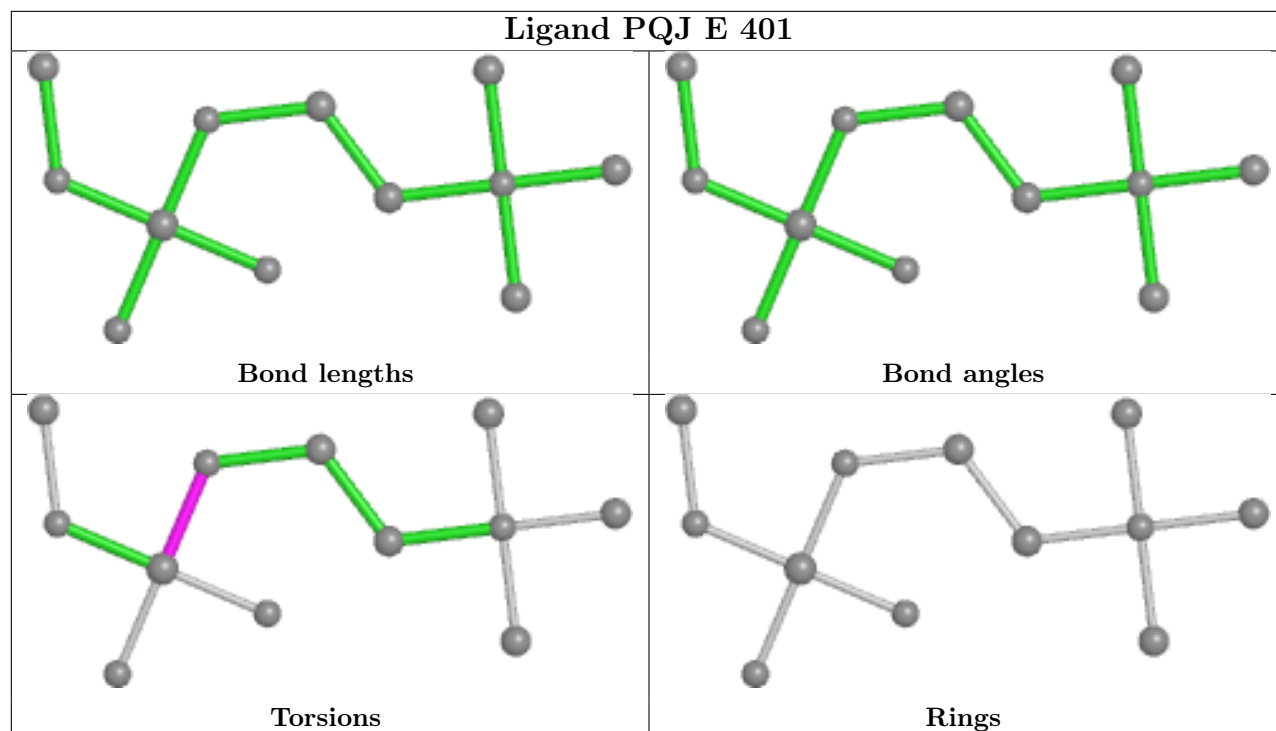
There are no ring outliers.

No monomer is involved in short contacts.

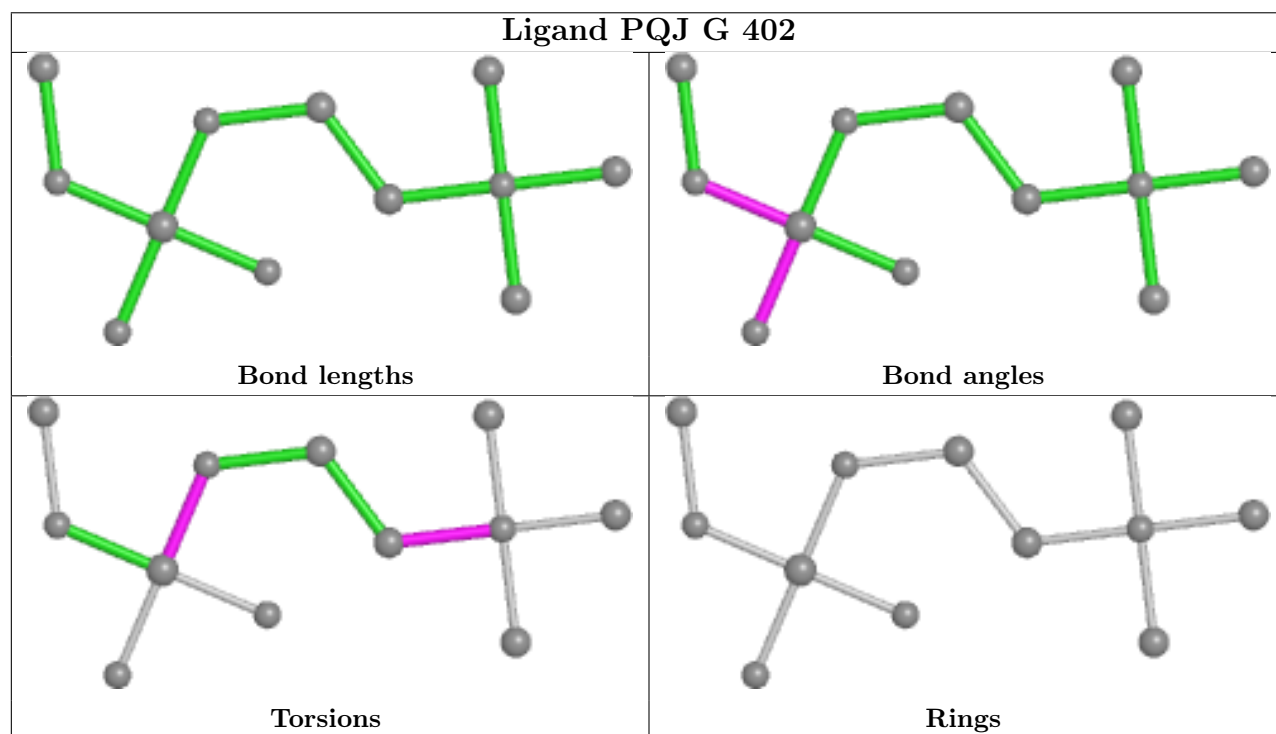
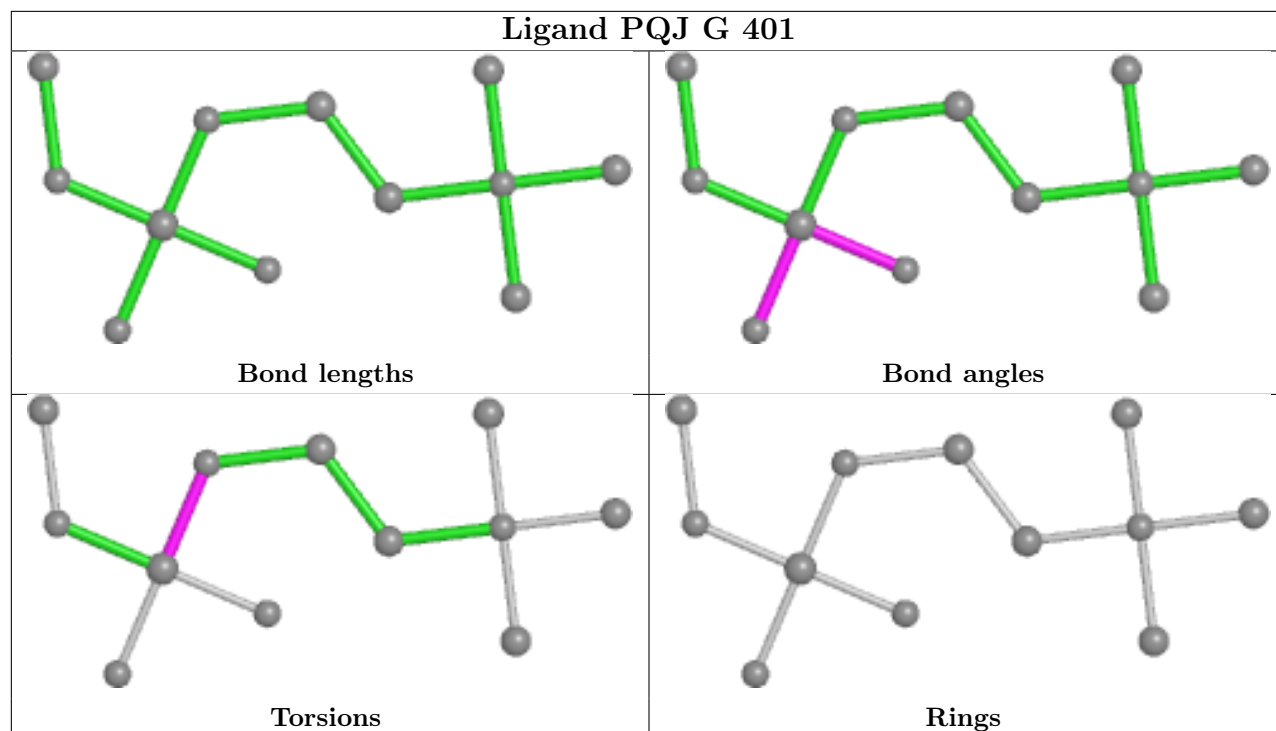
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

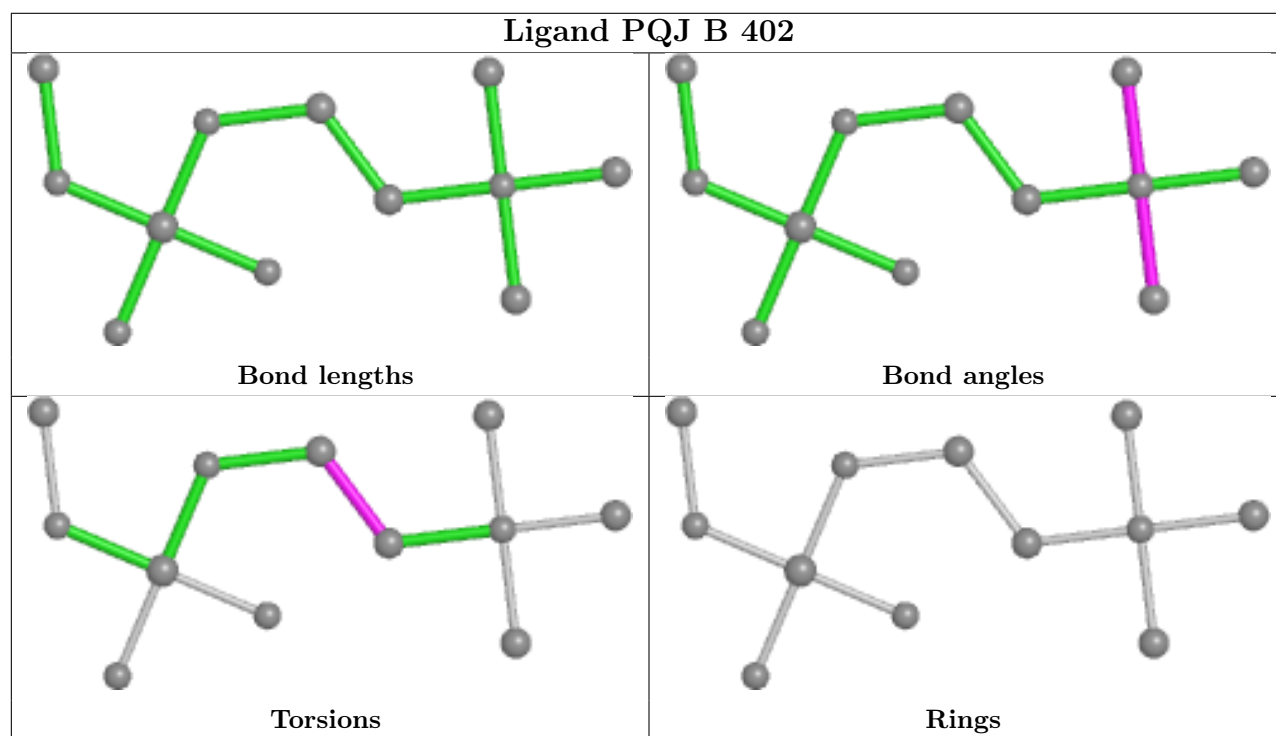
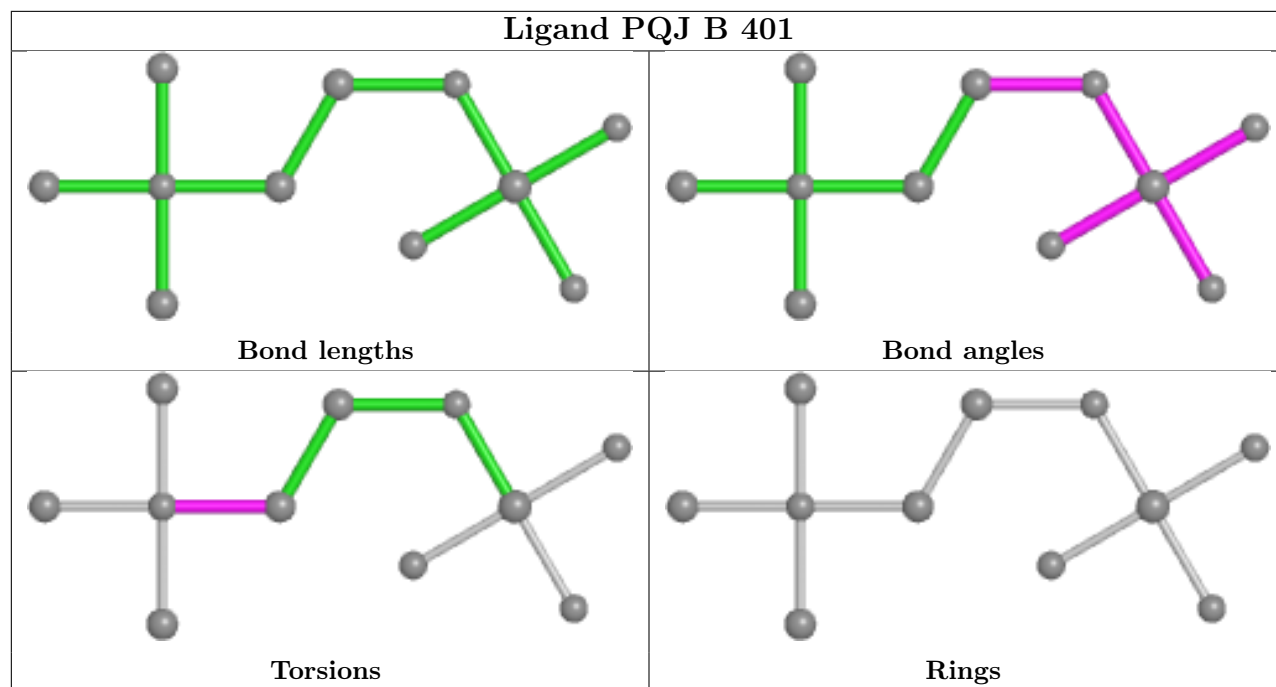


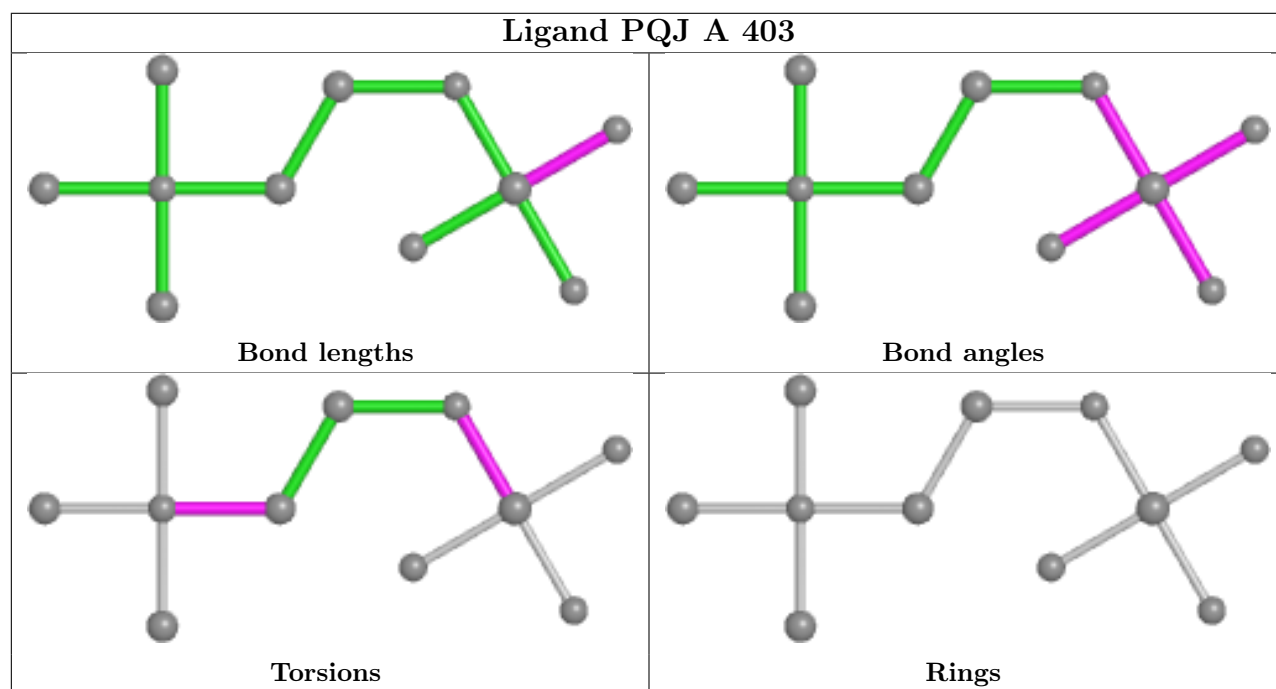
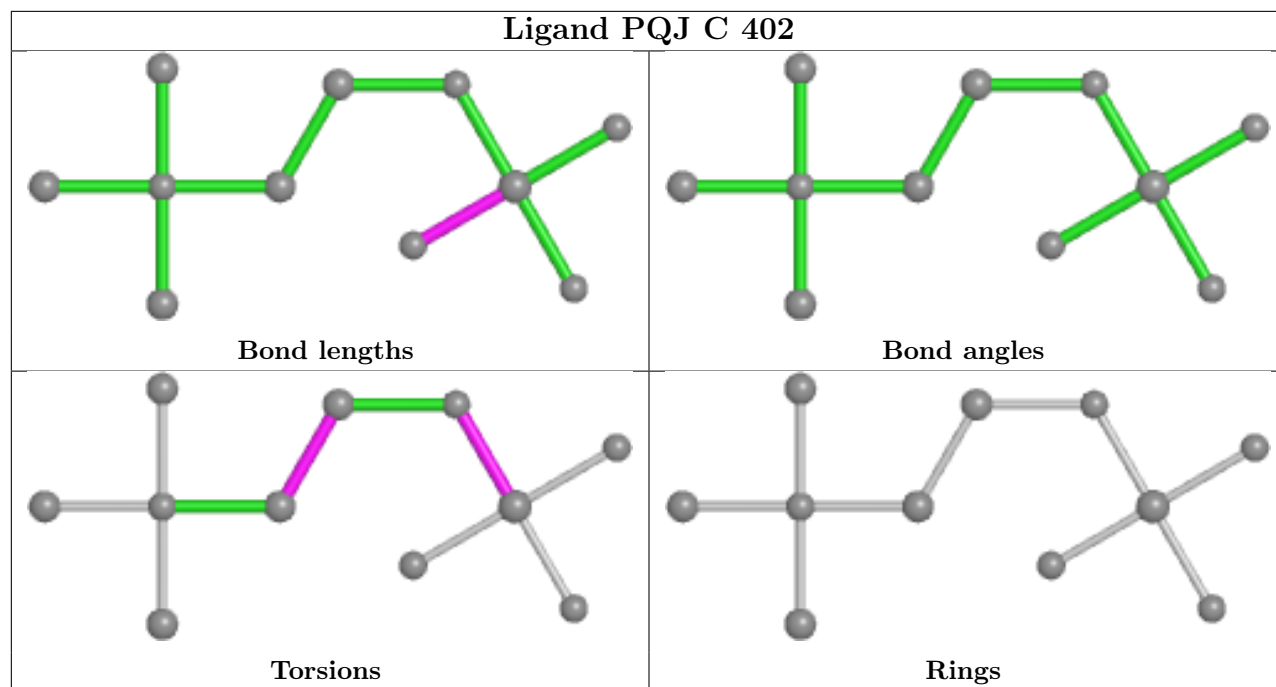


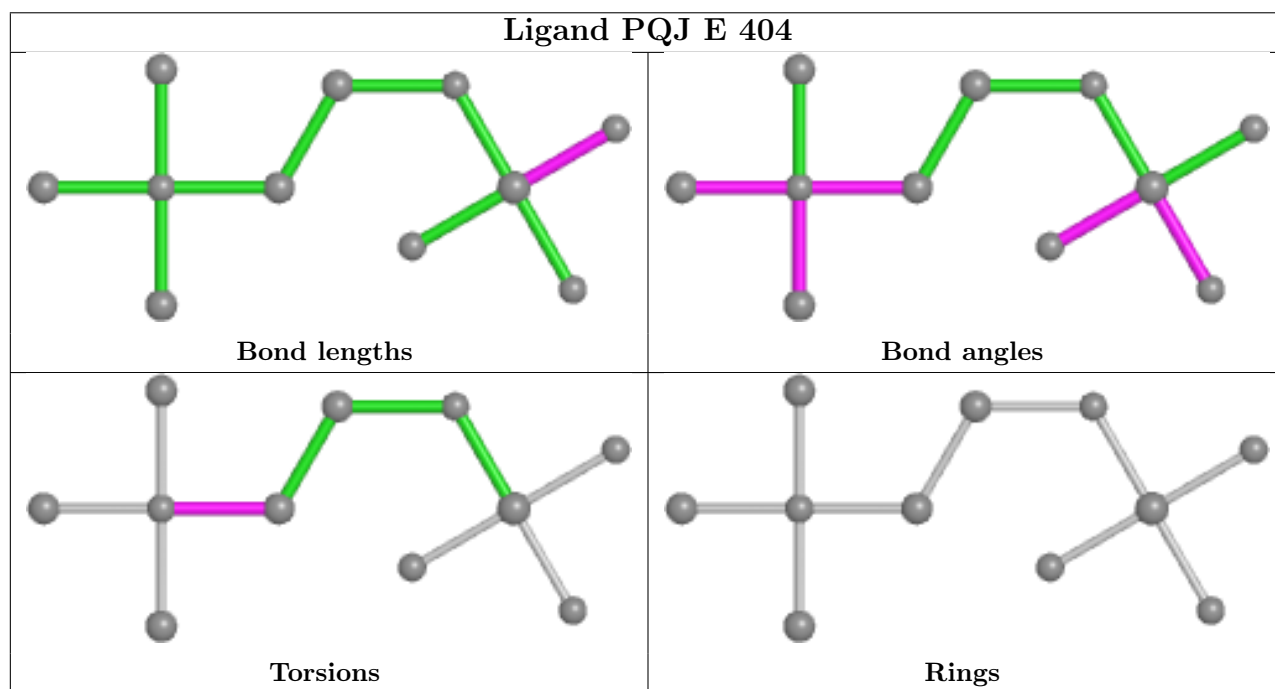
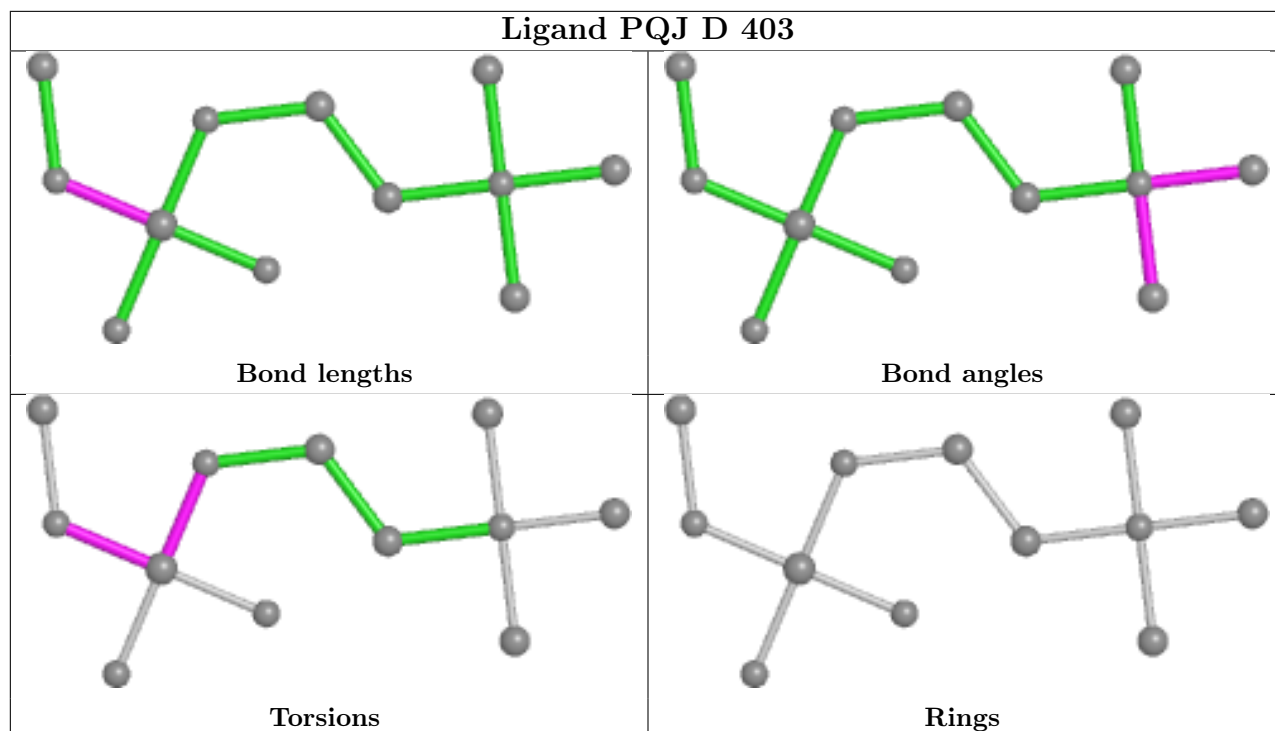


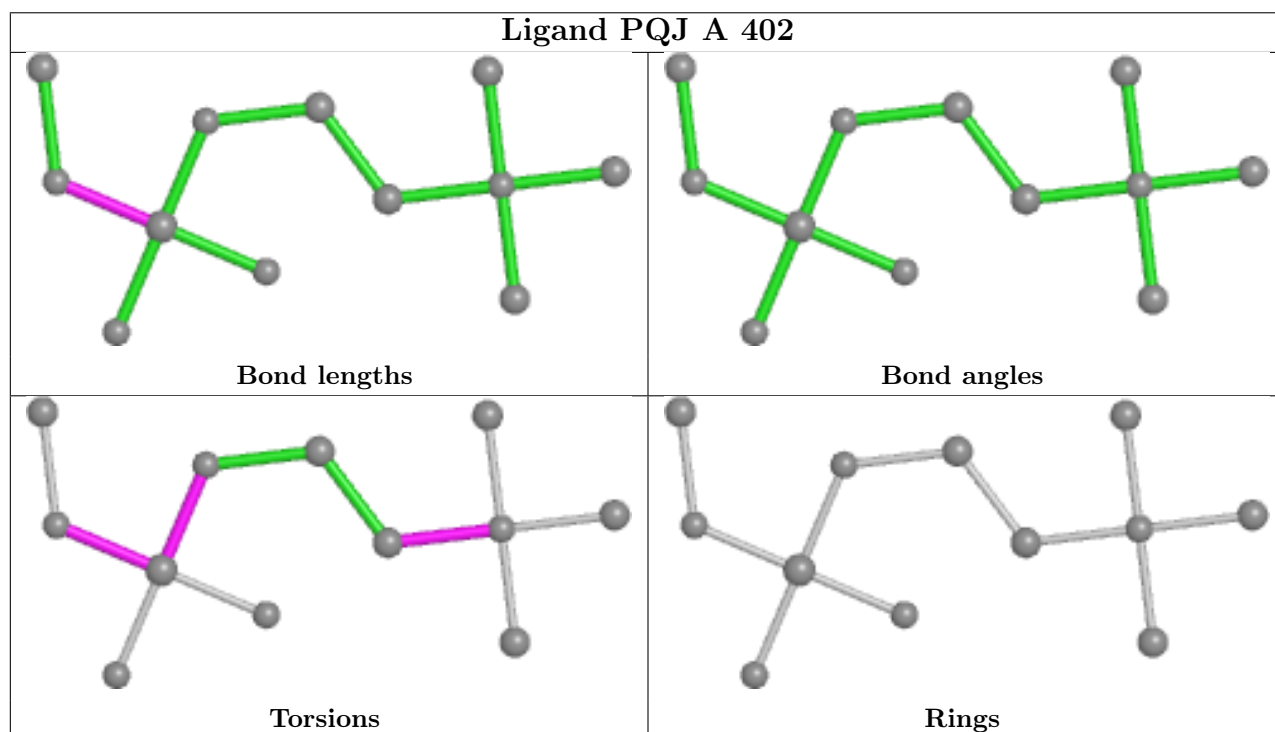
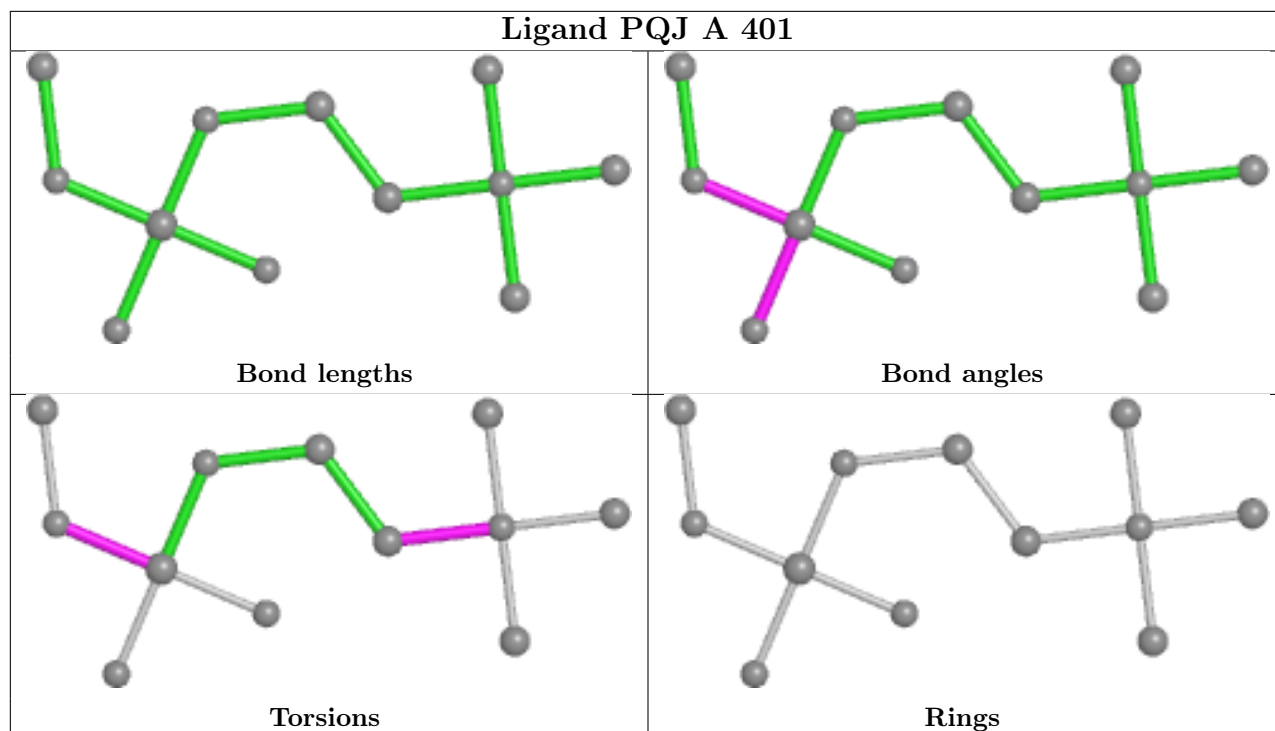


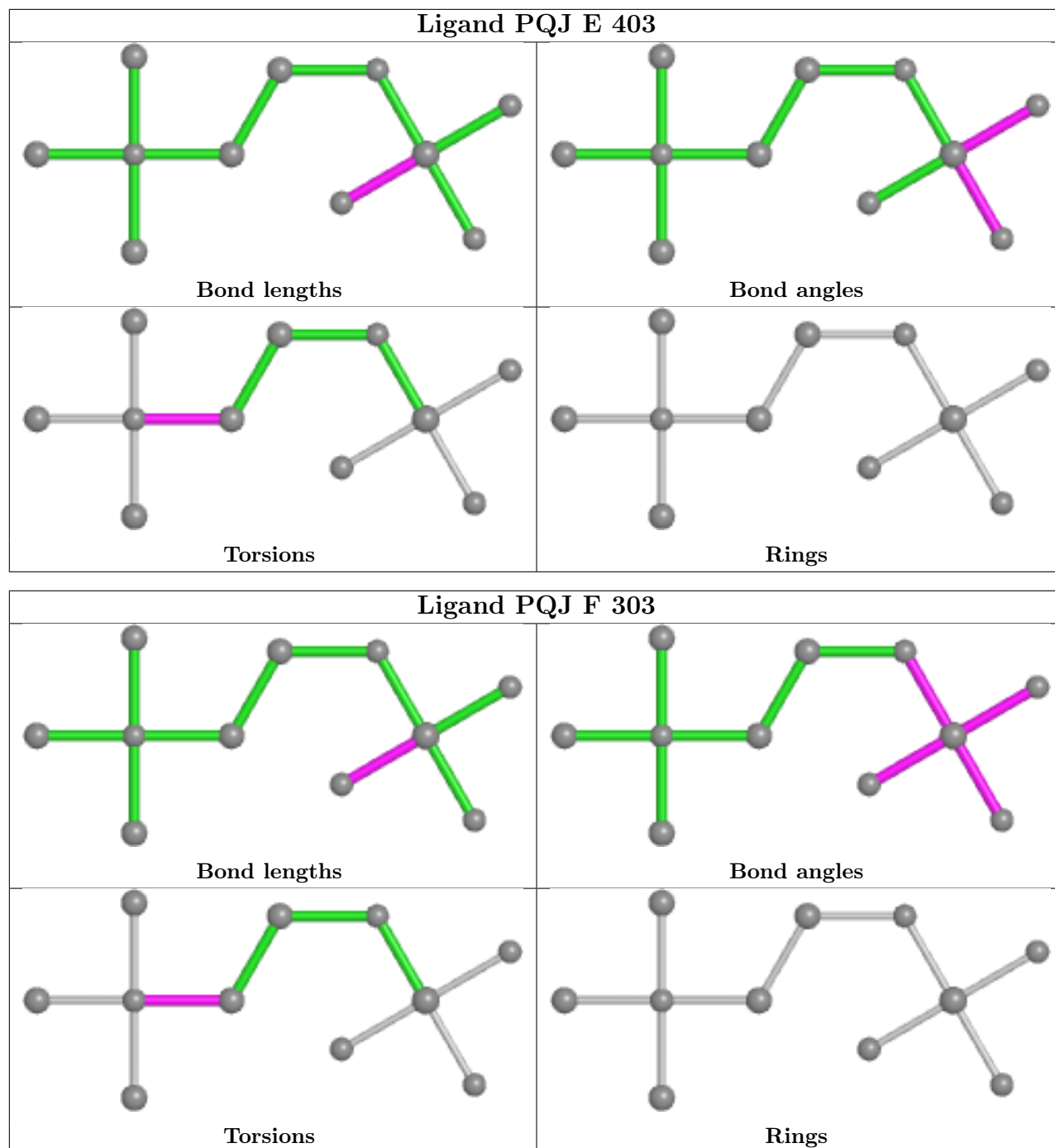


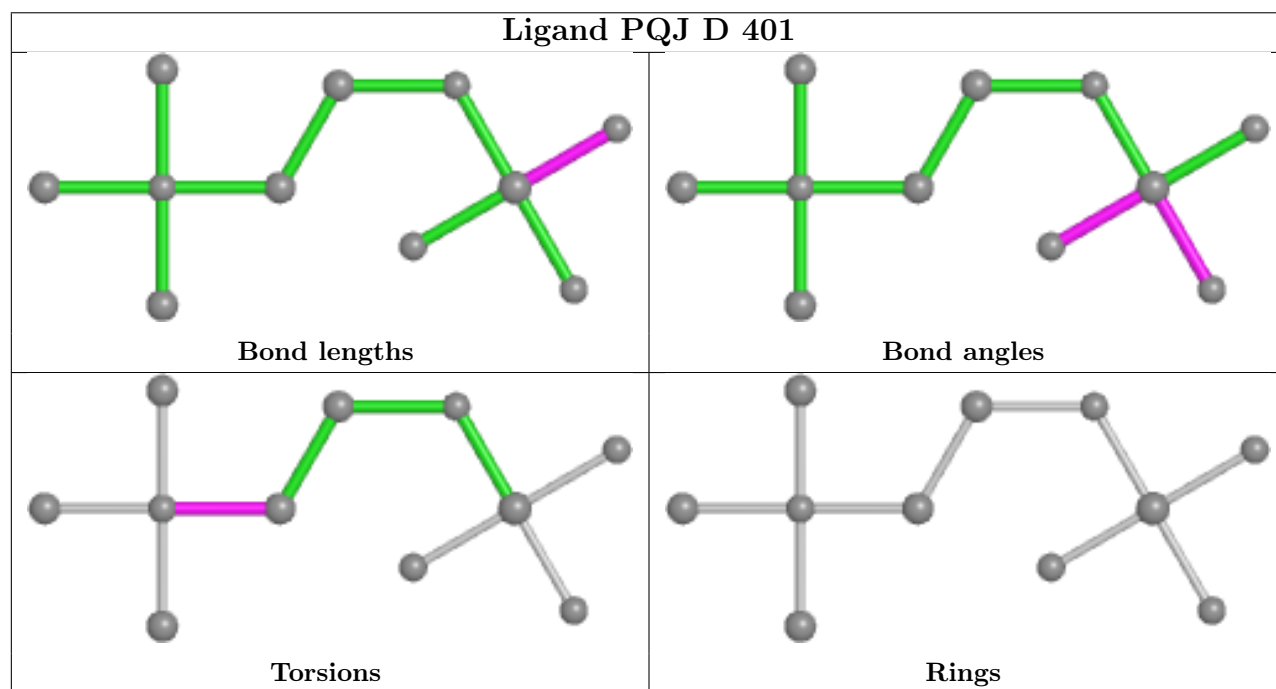
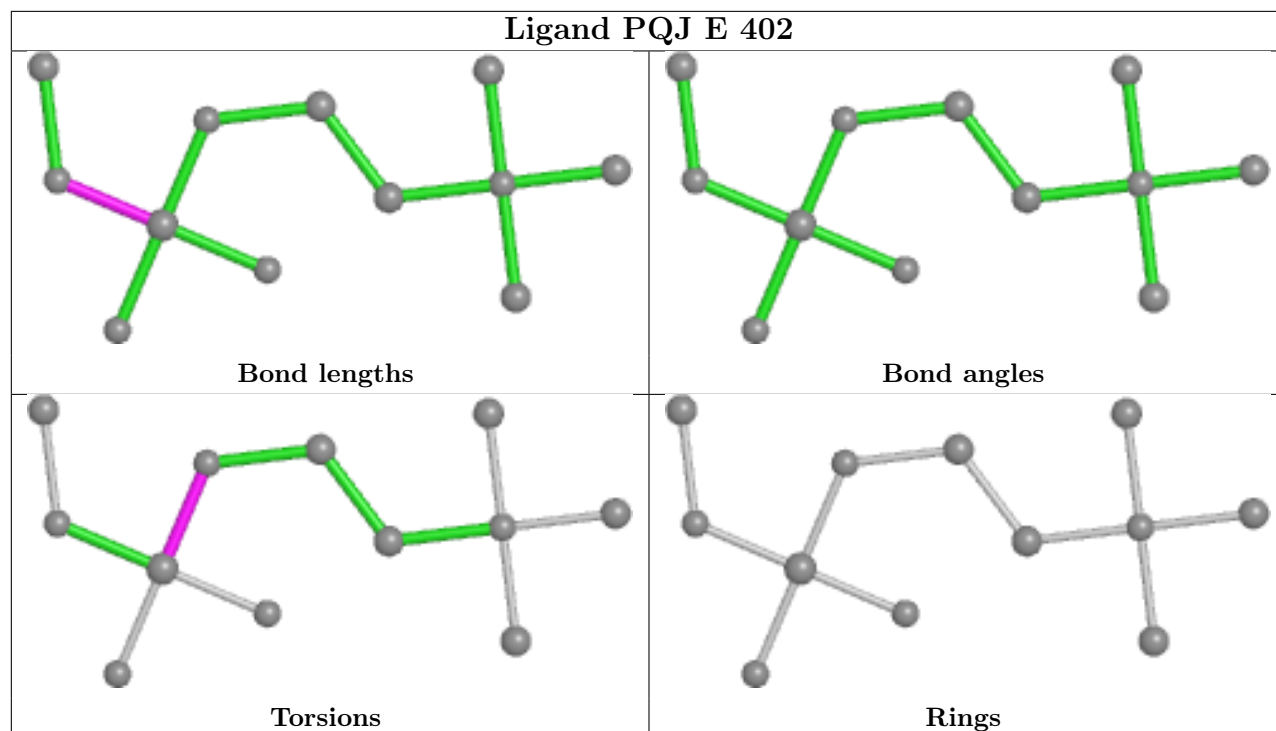


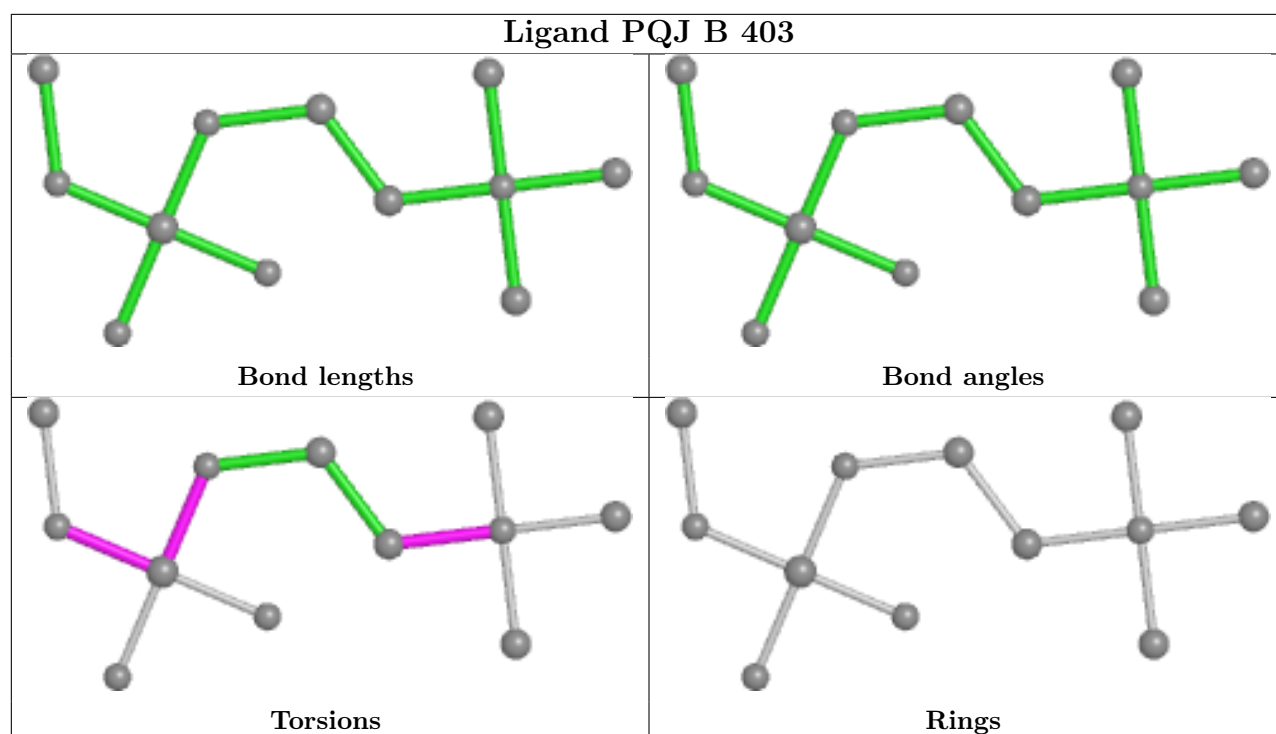












#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [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.