



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 06:45 PM EDT

PDB ID : 6PNX  
Title : Crystal Structure of an Asymmetric Dimer of FGF Receptor 3 Kinases Trapped in A-loop Tyrosine Transphosphorylation Reaction  
Authors : Mohammadi, M.  
Deposited on : 2019-07-03  
Resolution : 2.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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**  
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 2.20 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 4952 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 Fibroblast growth factor receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	291	2306	1470	395	423	18	0	1	0
1	B	294	2325	1481	398	428	18	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

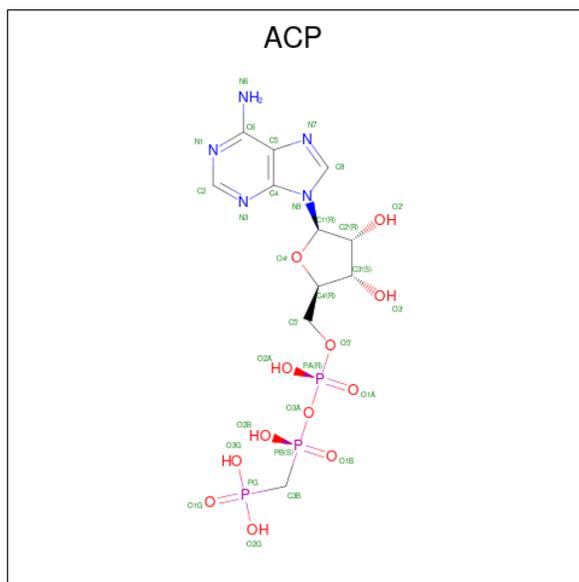
Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	expression tag	UNP P22607
A	437	GLY	-	expression tag	UNP P22607
A	438	SER	-	expression tag	UNP P22607
A	439	SER	-	expression tag	UNP P22607
A	440	HIS	-	expression tag	UNP P22607
A	441	HIS	-	expression tag	UNP P22607
A	442	HIS	-	expression tag	UNP P22607
A	443	HIS	-	expression tag	UNP P22607
A	444	HIS	-	expression tag	UNP P22607
A	445	HIS	-	expression tag	UNP P22607
A	446	SER	-	expression tag	UNP P22607
A	447	GLN	-	expression tag	UNP P22607
A	448	ASP	-	expression tag	UNP P22607
A	449	PRO	-	expression tag	UNP P22607
A	450	THR	-	expression tag	UNP P22607
A	482	ALA	CYS	engineered mutation	UNP P22607
A	582	SER	CYS	engineered mutation	UNP P22607
A	669	GLU	ARG	engineered mutation	UNP P22607
B	436	MET	-	expression tag	UNP P22607
B	437	GLY	-	expression tag	UNP P22607
B	438	SER	-	expression tag	UNP P22607
B	439	SER	-	expression tag	UNP P22607
B	440	HIS	-	expression tag	UNP P22607
B	441	HIS	-	expression tag	UNP P22607
B	442	HIS	-	expression tag	UNP P22607

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Chain	Residue	Modelled	Actual	Comment	Reference
B	443	HIS	-	expression tag	UNP P22607
B	444	HIS	-	expression tag	UNP P22607
B	445	HIS	-	expression tag	UNP P22607
B	446	SER	-	expression tag	UNP P22607
B	447	GLN	-	expression tag	UNP P22607
B	448	ASP	-	expression tag	UNP P22607
B	449	PRO	-	expression tag	UNP P22607
B	450	THR	-	expression tag	UNP P22607
B	482	ALA	CYS	engineered mutation	UNP P22607
B	582	SER	CYS	engineered mutation	UNP P22607
B	669	GLU	ARG	engineered mutation	UNP P22607

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	106	Total	O	0	0
			106	106		

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.69Å 93.25Å 75.49Å 90.00° 103.06° 90.00°	Depositor
Resolution (Å)	39.38 – 2.20	Depositor
% Data completeness (in resolution range)	99.6 (39.38-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.80 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.193 , 0.230	Depositor
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtrriage
Anisotropy	0.244	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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](#)

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### 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](#)

4 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

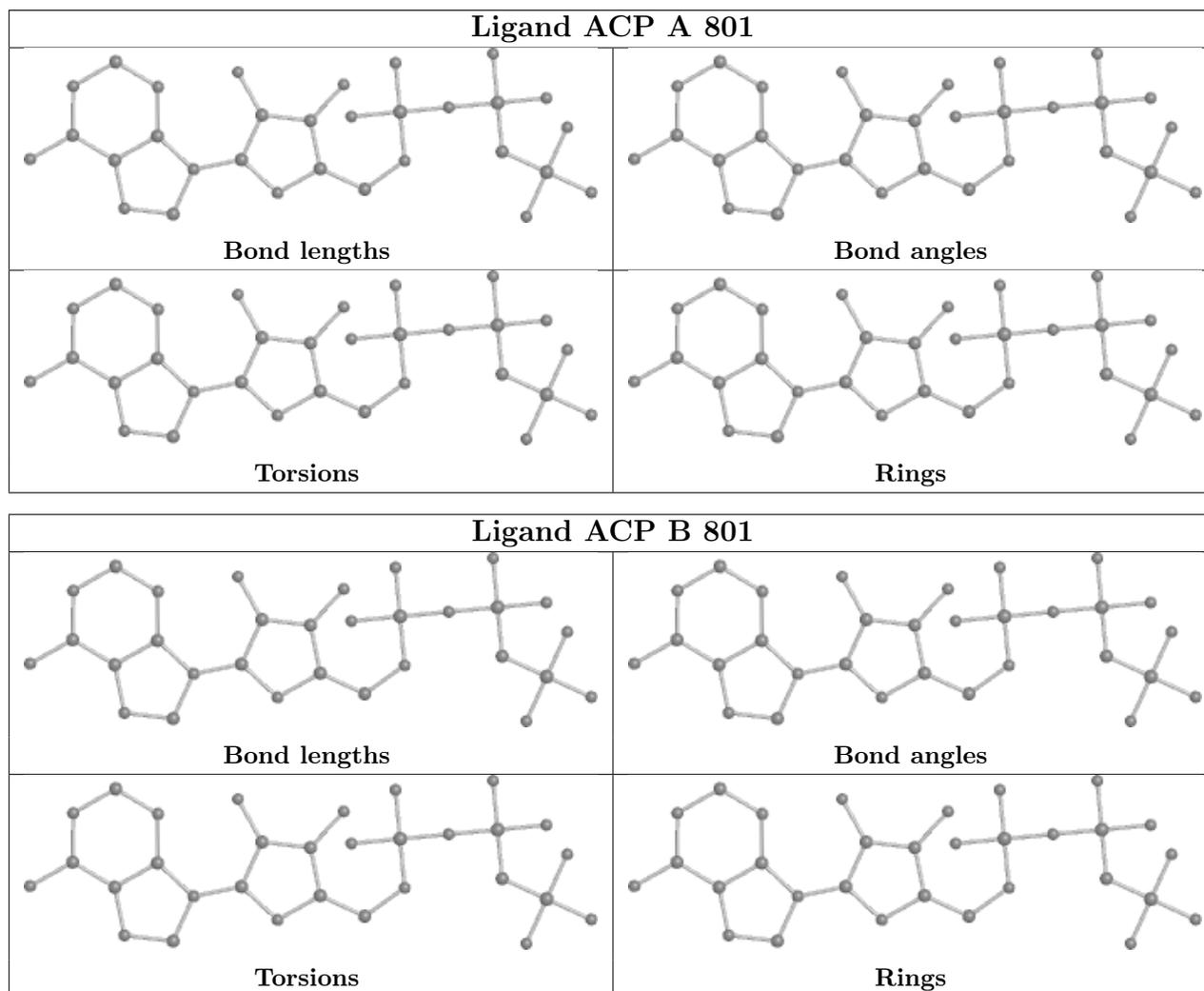
There are no chirality outliers.

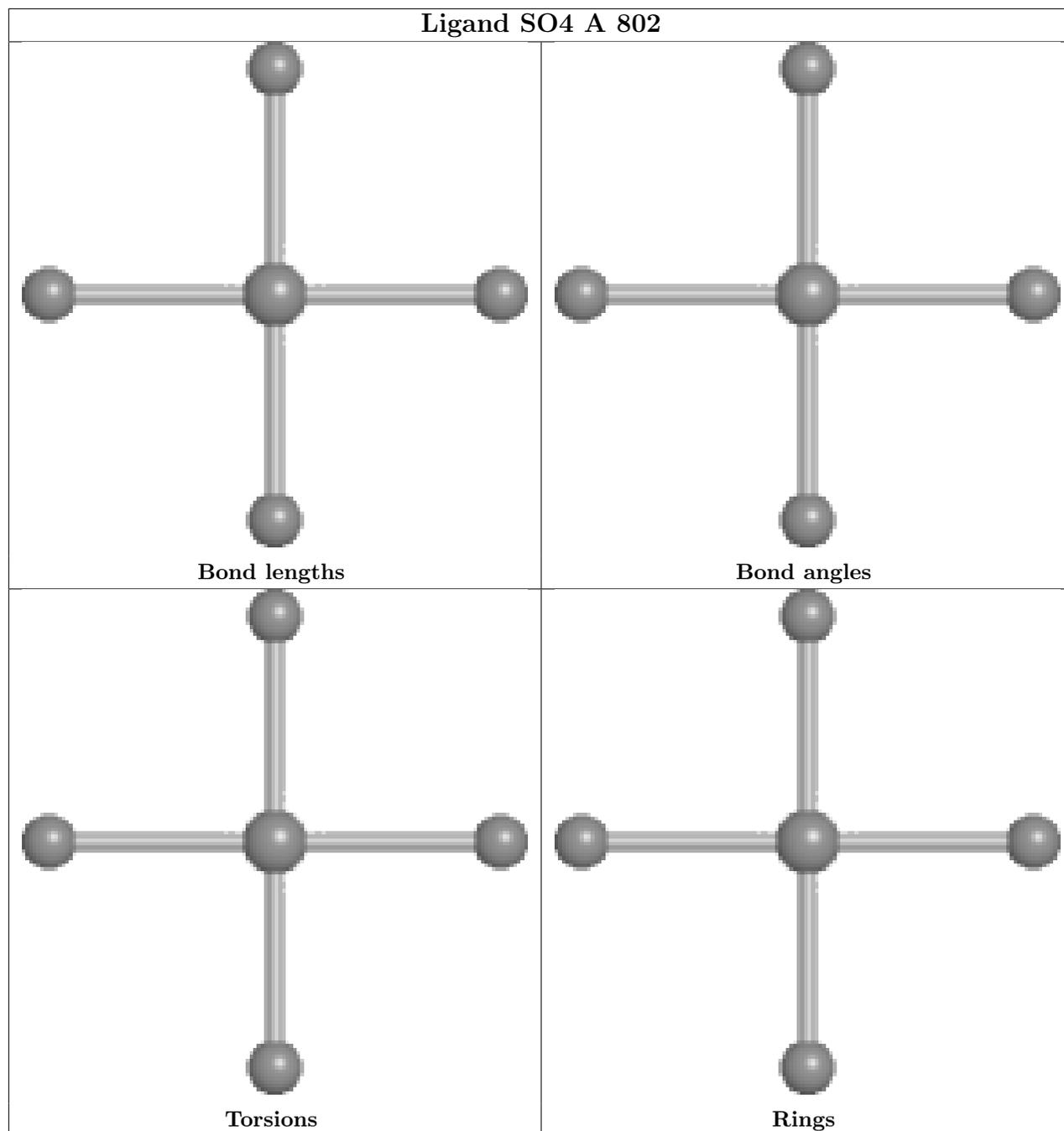
There are no torsion outliers.

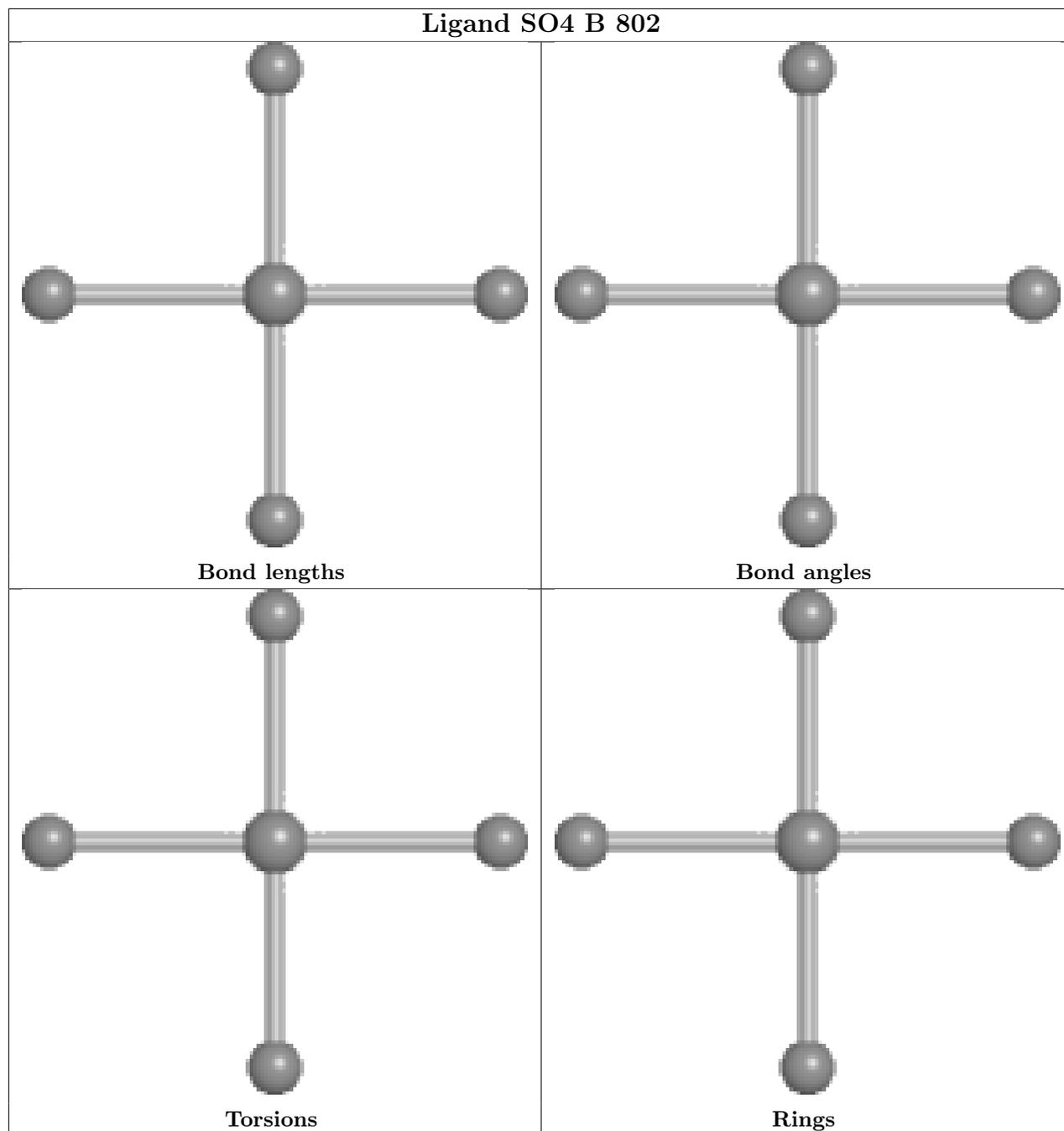
There are no ring outliers.

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 [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.