



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:48 PM EDT

PDB ID : 6NTT
Title : X-ray Crystal Structure of Soybean Trypsin Inhibitor (Kunitz) Complexed with 1,5-Disulfonyl Naphthalene
Authors : McPherson, A.
Deposited on : 2019-01-30
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)
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 2.40 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](#)

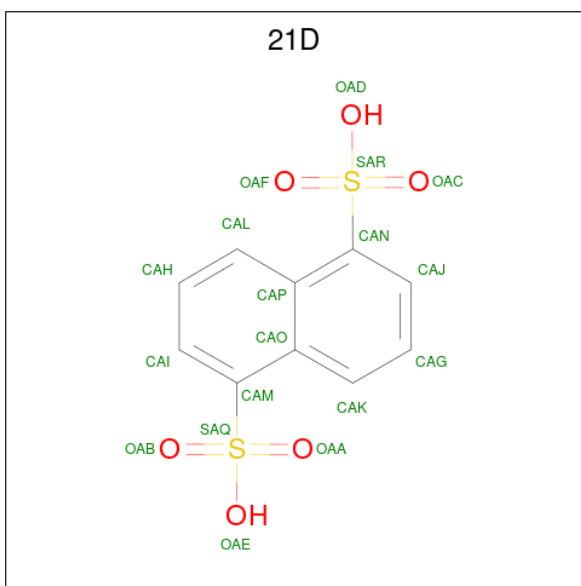
There are 4 unique types of molecules in this entry. The entry contains 3130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Trypsin inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	Total 1376	C 871	N 232	O 267	S 6	0	2	0
1	B	176	Total 1373	C 868	N 232	O 267	S 6	0	0	0

- Molecule 2 is naphthalene-1,5-disulfonic acid (three-letter code: 21D) (formula: C₁₀H₈O₆S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	Total 36	C 20	O 12	S 4	0	1
2	B	1	Total 36	C 20	O 12	S 4	0	1
2	B	1	Total 36	C 20	O 12	S 4	0	1

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	24	12	2	8	2	0	1
3	B	1	12	6	1	4	1	0	0
3	B	1	12	6	1	4	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	123	123	123	0	0
4	B	102	102	102	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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.88Å 64.68Å 69.08Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	32.61 – 2.40	Depositor
% Data completeness (in resolution range)	93.2 (32.61-2.40)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.306	Depositor
Wilson B-factor (Å ²)	42.1	Xtrriage
Anisotropy	0.384	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3130	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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](#)

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](#)

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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](#)

10 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
2	21D	B	202[A]	-	17,19,19	0.33	0	24,30,30	0.15	0
3	MES	A	202[A]	-	12,12,12	0.70	0	14,16,16	0.41	0
2	21D	B	201[B]	-	17,19,19	0.44	0	24,30,30	0.18	0
2	21D	A	201[A]	-	17,19,19	0.31	0	24,30,30	0.25	0
2	21D	B	202[B]	-	17,19,19	0.33	0	24,30,30	0.22	0
3	MES	B	203	-	12,12,12	0.74	0	14,16,16	0.39	0
3	MES	B	204	-	12,12,12	0.75	0	14,16,16	0.36	0
3	MES	A	202[B]	-	12,12,12	0.76	0	14,16,16	0.44	0
2	21D	B	201[A]	-	17,19,19	0.22	0	24,30,30	0.15	0
2	21D	A	201[B]	-	17,19,19	0.42	0	24,30,30	0.23	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	21D	B	202[A]	-	-	0/12/12/12	0/2/2/2
3	MES	A	202[A]	-	-	5/6/14/14	0/1/1/1
2	21D	B	201[B]	-	-	6/12/12/12	0/2/2/2
2	21D	A	201[A]	-	-	12/12/12/12	0/2/2/2
2	21D	B	202[B]	-	-	6/12/12/12	0/2/2/2
3	MES	B	203	-	-	3/6/14/14	0/1/1/1
3	MES	B	204	-	-	3/6/14/14	0/1/1/1
3	MES	A	202[B]	-	-	6/6/14/14	0/1/1/1
2	21D	B	201[A]	-	-	5/12/12/12	0/2/2/2
2	21D	A	201[B]	-	-	11/12/12/12	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201[A]	21D	CAI-CAM-SAQ-OAA

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Mol	Chain	Res	Type	Atoms
2	A	201[A]	21D	CAO-CAM-SAQ-OAA
2	A	201[A]	21D	CAI-CAM-SAQ-OAB
2	A	201[A]	21D	CAO-CAM-SAQ-OAB
2	A	201[A]	21D	CAP-CAN-SAR-OAF
2	A	201[A]	21D	CAP-CAN-SAR-OAC
2	A	201[A]	21D	CAJ-CAN-SAR-OAF
2	A	201[A]	21D	CAJ-CAN-SAR-OAC
2	A	201[B]	21D	CAI-CAM-SAQ-OAA
2	A	201[B]	21D	CAO-CAM-SAQ-OAA
2	A	201[B]	21D	CAI-CAM-SAQ-OAB
2	A	201[B]	21D	CAO-CAM-SAQ-OAB
2	A	201[B]	21D	CAP-CAN-SAR-OAD
2	B	201[A]	21D	CAI-CAM-SAQ-OAE
2	B	201[A]	21D	CAI-CAM-SAQ-OAA
2	B	201[A]	21D	CAO-CAM-SAQ-OAA
2	B	201[A]	21D	CAI-CAM-SAQ-OAB
2	B	201[A]	21D	CAO-CAM-SAQ-OAB
2	B	201[B]	21D	CAO-CAM-SAQ-OAE
2	B	201[B]	21D	CAI-CAM-SAQ-OAA
2	B	201[B]	21D	CAO-CAM-SAQ-OAB
3	A	202[A]	MES	C8-C7-N4-C5
3	A	202[A]	MES	N4-C7-C8-S
3	A	202[A]	MES	C7-C8-S-O1S
3	A	202[A]	MES	C7-C8-S-O3S
3	A	202[B]	MES	C8-C7-N4-C5
3	A	202[B]	MES	N4-C7-C8-S
3	A	202[B]	MES	C7-C8-S-O2S
3	A	202[B]	MES	C7-C8-S-O3S
3	B	203	MES	C8-C7-N4-C5
3	B	204	MES	C8-C7-N4-C3
3	B	204	MES	N4-C7-C8-S
2	A	201[B]	21D	CAP-CAN-SAR-OAF
2	A	201[B]	21D	CAP-CAN-SAR-OAC
2	B	201[B]	21D	CAO-CAM-SAQ-OAA
2	B	202[B]	21D	CAP-CAN-SAR-OAF
2	B	202[B]	21D	CAP-CAN-SAR-OAC
2	A	201[B]	21D	CAJ-CAN-SAR-OAF
2	B	201[B]	21D	CAI-CAM-SAQ-OAB
2	B	202[B]	21D	CAJ-CAN-SAR-OAF
3	B	203	MES	N4-C7-C8-S
3	B	203	MES	C8-C7-N4-C3
3	B	204	MES	C8-C7-N4-C5

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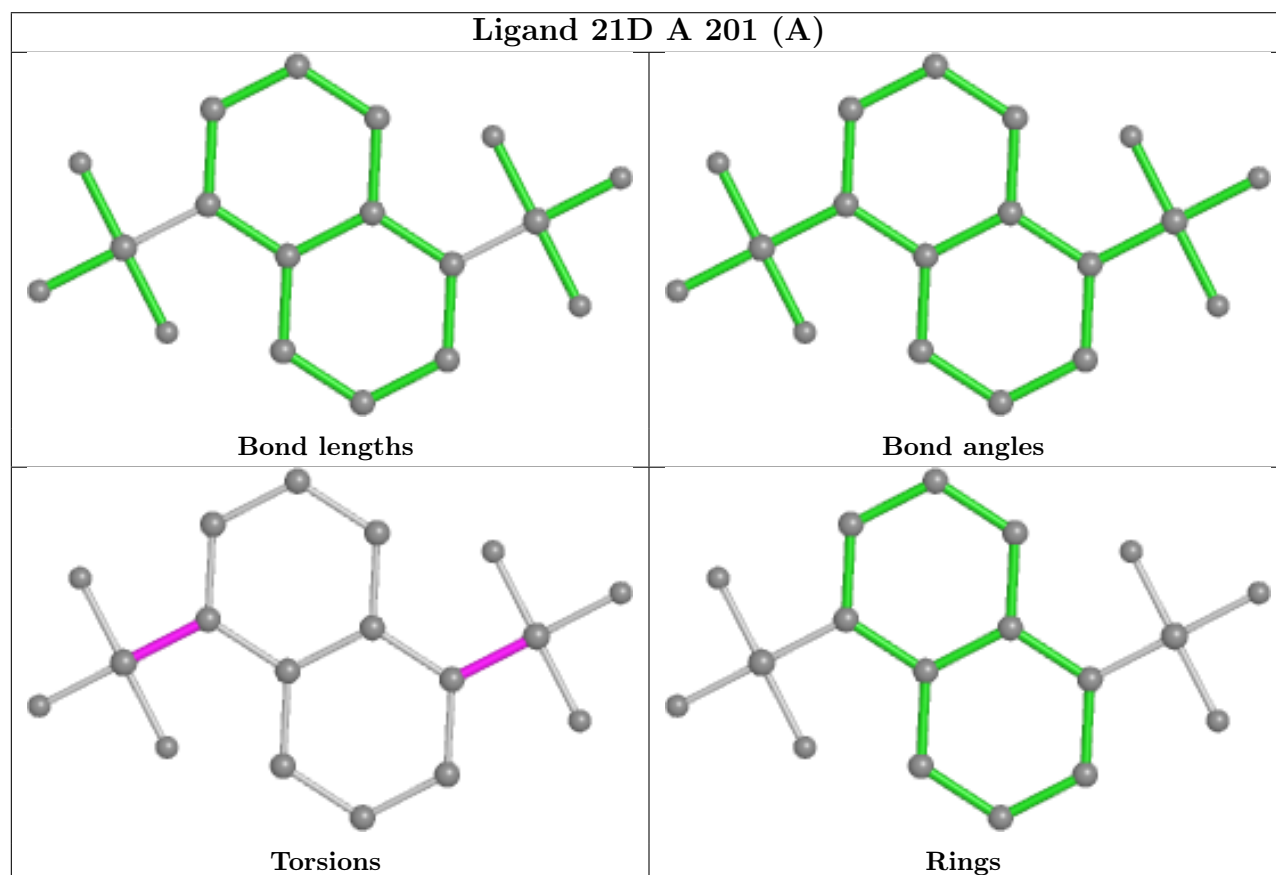
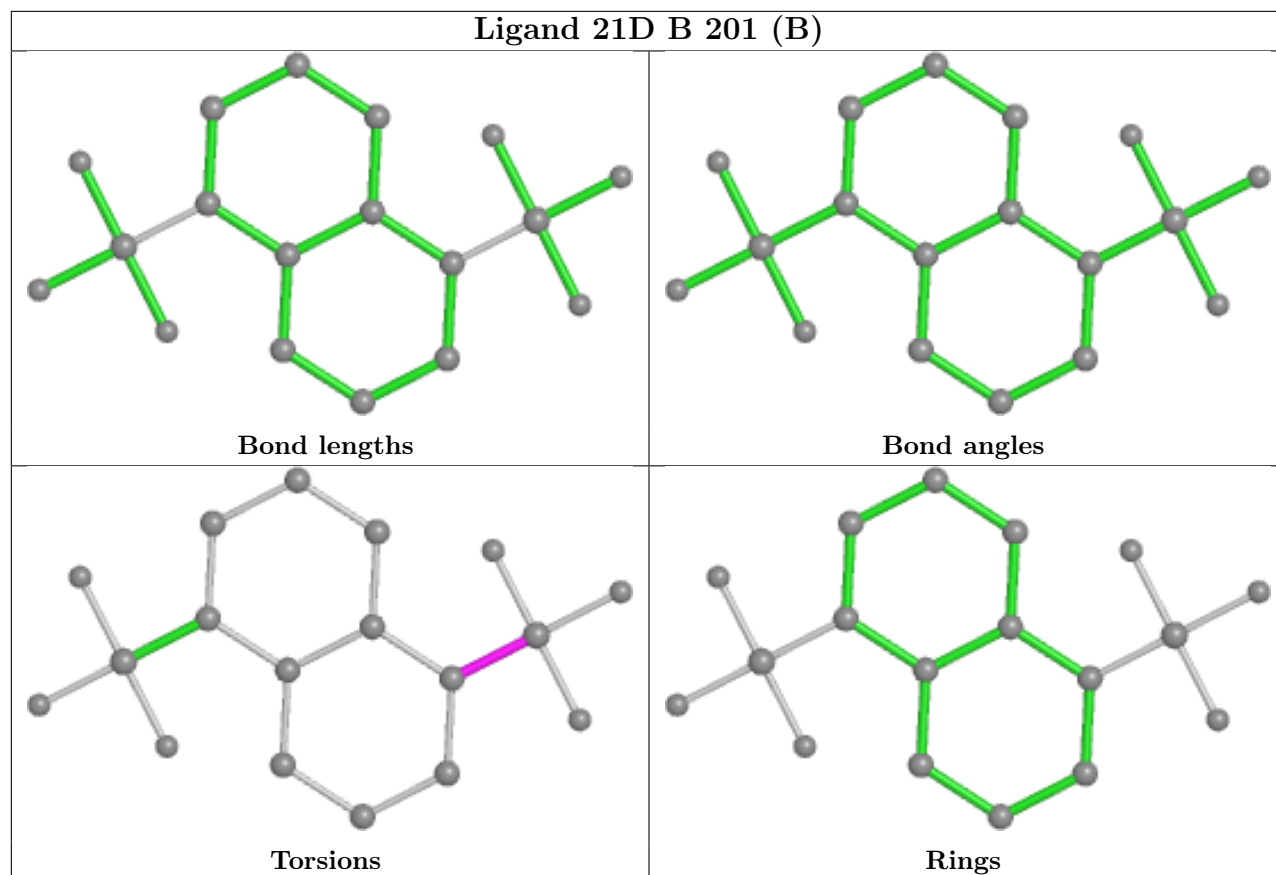
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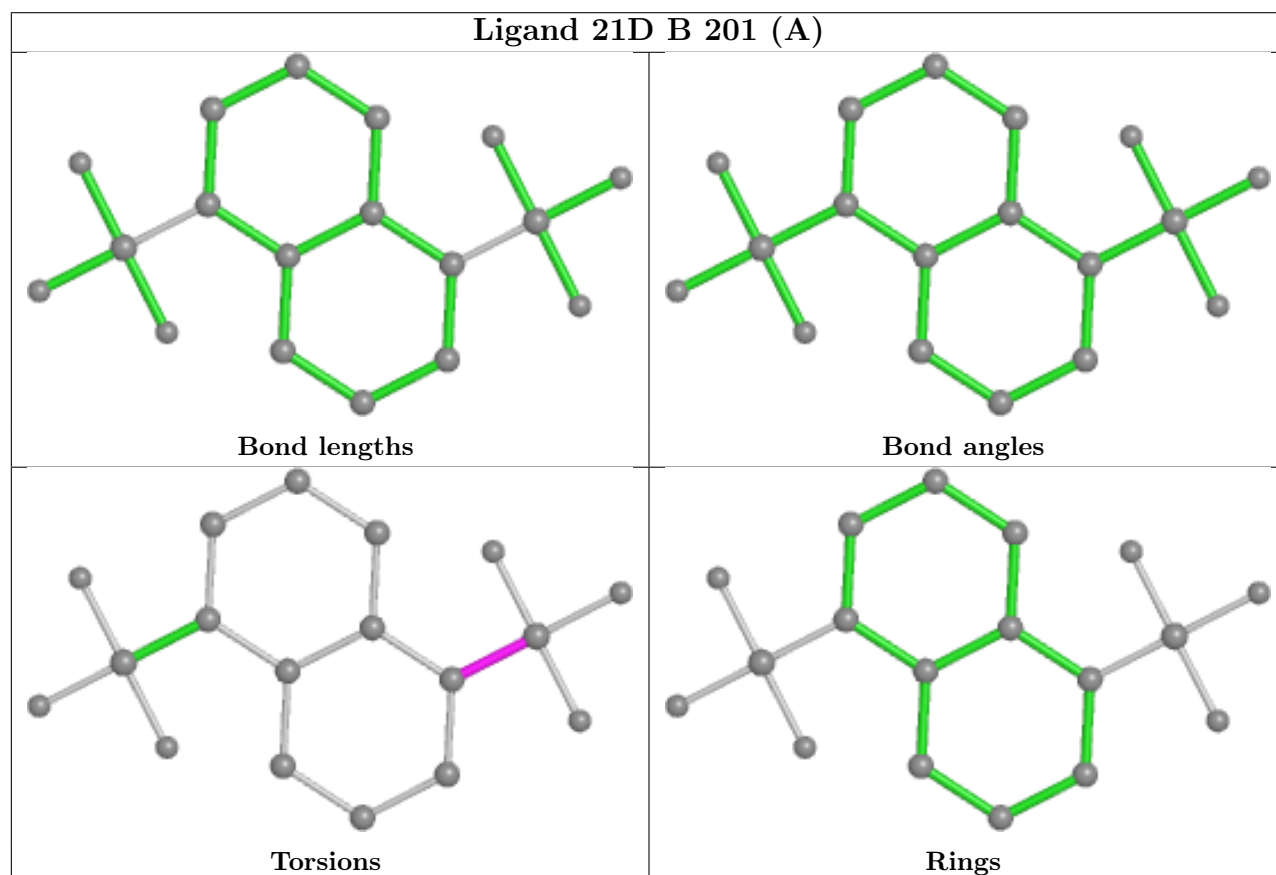
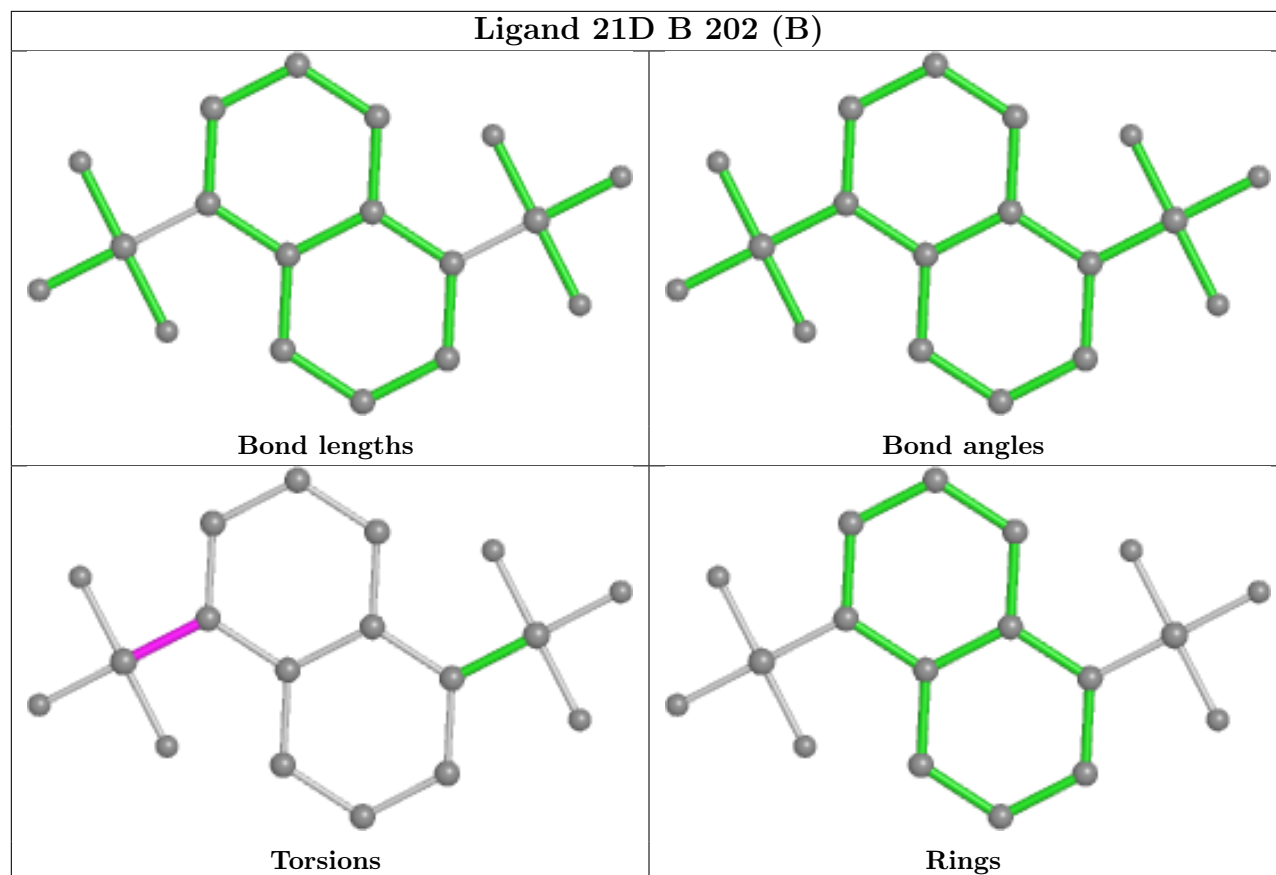
Mol	Chain	Res	Type	Atoms
3	A	202[A]	MES	C7-C8-S-O2S
3	A	202[B]	MES	C7-C8-S-O1S
2	A	201[A]	21D	CAI-CAM-SAQ-OAE
2	A	201[A]	21D	CAO-CAM-SAQ-OAE
2	A	201[A]	21D	CAP-CAN-SAR-OAD
2	A	201[A]	21D	CAJ-CAN-SAR-OAD
2	A	201[B]	21D	CAI-CAM-SAQ-OAE
2	A	201[B]	21D	CAO-CAM-SAQ-OAE
2	B	201[B]	21D	CAI-CAM-SAQ-OAE
2	B	202[B]	21D	CAP-CAN-SAR-OAD
2	B	202[B]	21D	CAJ-CAN-SAR-OAD
2	A	201[B]	21D	CAJ-CAN-SAR-OAC
2	B	202[B]	21D	CAJ-CAN-SAR-OAC
3	A	202[B]	MES	C8-C7-N4-C3

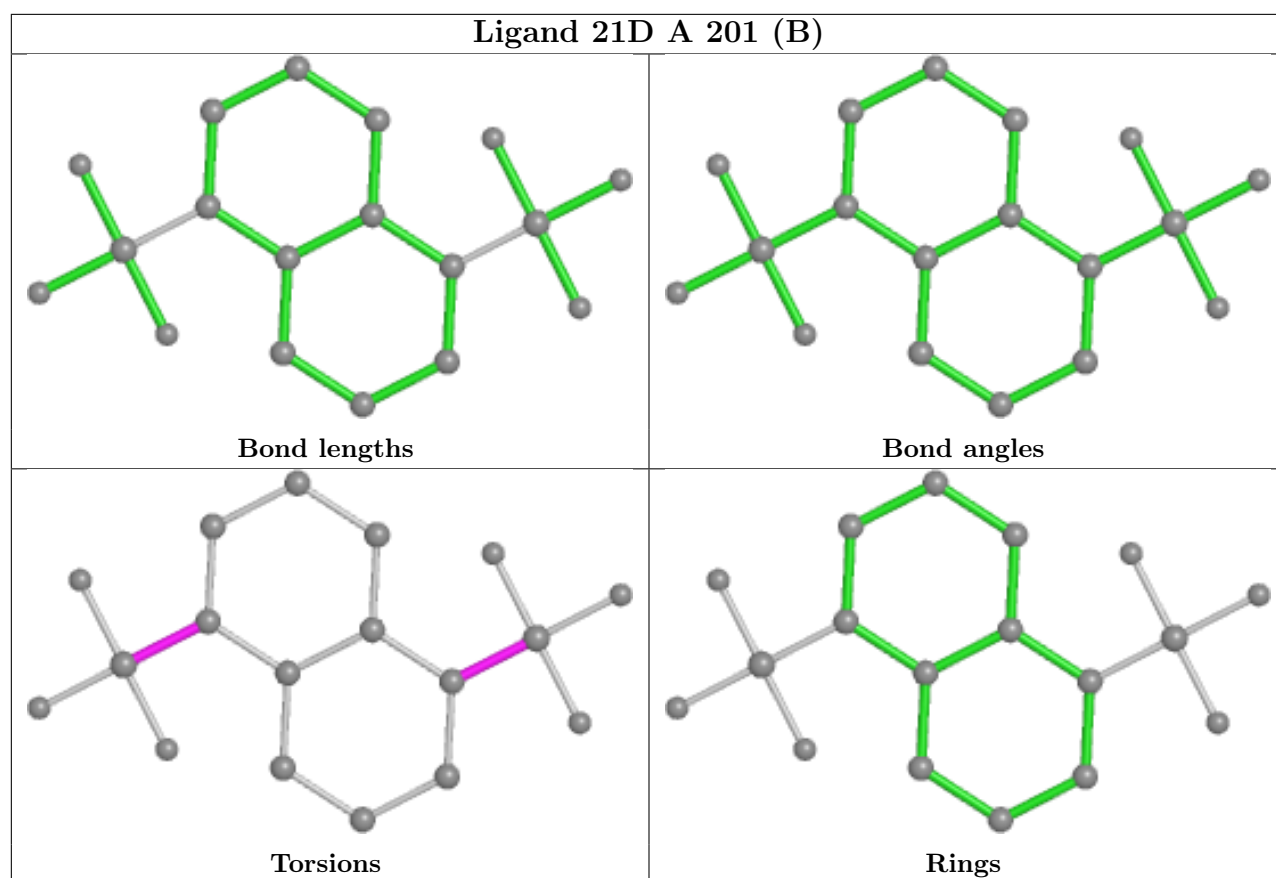
There are no ring outliers.

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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	138:GLN	C	139:GLN	N	13.79

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.