



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 03:21 AM EDT

PDB ID : 6VSG  
Title : Mycobacterium tuberculosis dihydrofolate reductase in complex with 4-(trifluoromethyl)benzene-1,2-diamine(fragment 17)  
Authors : Ribeiro, J.A.; Dias, M.V.B.  
Deposited on : 2020-02-11  
Resolution : 2.30 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 2.30 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 6 unique types of molecules in this entry. The entry contains 2800 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.

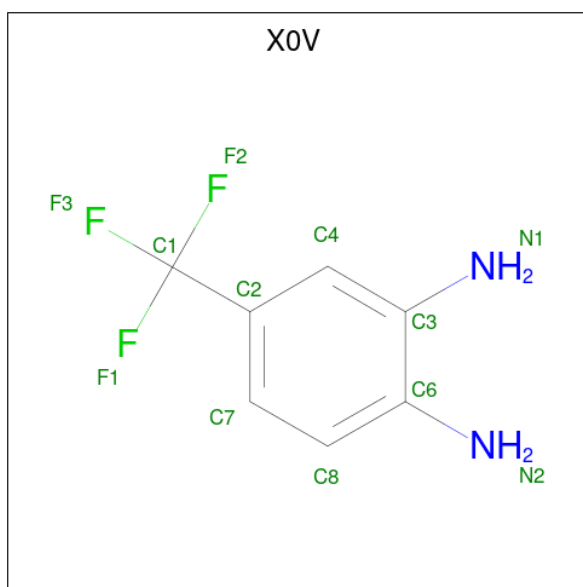
- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	Total	C	N	O	S	0	0	0
			1240	781	228	226	5			
1	B	159	Total	C	N	O	S	0	0	0
			1244	783	228	228	5			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

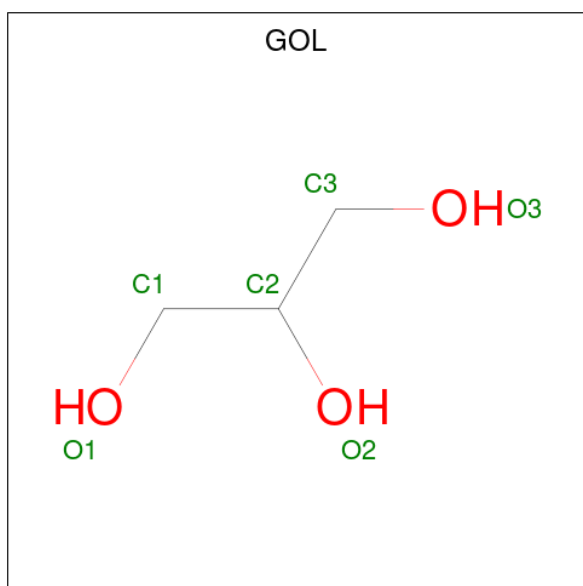
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		

- Molecule 3 is 4-(TRIFLUOROMETHYL)BENZENE-1,2-DIAMINE (three-letter code: X0V) (formula: C<sub>7</sub>H<sub>7</sub>F<sub>3</sub>N<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



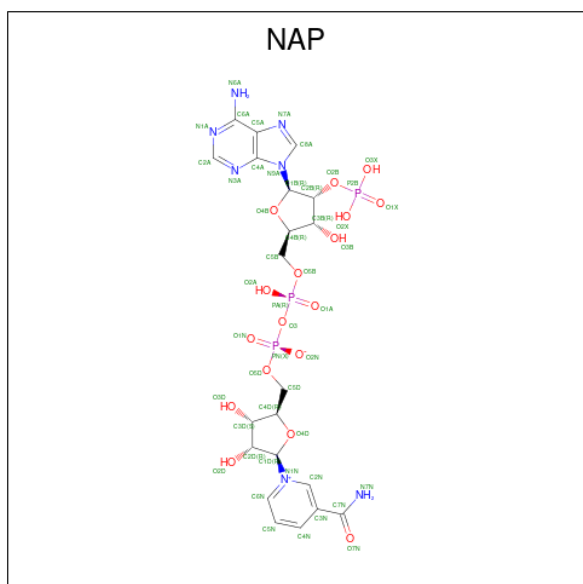
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
3	A	1	Total	C	F	N	0	0
			12	7	3	2		

- 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	0	0
			6	3	3		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	48	21	7	17	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total 90	O 90	0	0
6	B	110	Total 110	O 110	0	0

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	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.91Å 70.70Å 72.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.54 – 2.30	Depositor
% Data completeness (in resolution range)	99.2 (46.54-2.30)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.32Å)	Xtrriage
Refinement program	PHENIX 1.14	Depositor
R, $R_{free}$	0.170 , 0.222	Depositor
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.285	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.086 for -h,l,k	Xtrriage
Reported twinning fraction	0.060 for -h,l,k	Depositor
Outliers	0 of 14181 reflections	Xtrriage
Total number of atoms	2800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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](#)

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### 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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	NAP	A	205	-	45,52,52	2.48	12 (26%)	56,80,80	1.98	14 (25%)
3	X0V	A	203	-	12,12,12	1.29	2 (16%)	17,18,18	1.16	2 (11%)
4	GOL	A	204	-	5,5,5	0.41	0	5,5,5	0.42	0
5	NAP	B	201	-	45,52,52	2.53	12 (26%)	56,80,80	1.98	17 (30%)

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
5	NAP	A	205	-	-	4/31/67/67	0/5/5/5
3	X0V	A	203	-	-	0/6/6/6	0/1/1/1
4	GOL	A	204	-	-	0/4/4/4	-
5	NAP	B	201	-	-	6/31/67/67	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	NAP	P2B-O2B	11.11	1.80	1.59
5	A	205	NAP	P2B-O2B	11.06	1.80	1.59
5	A	205	NAP	C4N-C3N	5.42	1.48	1.39
5	B	201	NAP	C4N-C3N	5.28	1.48	1.39
5	B	201	NAP	C5N-C4N	4.83	1.49	1.38
5	A	205	NAP	C5N-C4N	4.56	1.48	1.38
5	A	205	NAP	PN-O5D	4.53	1.77	1.59
5	A	205	NAP	C3N-C7N	-4.18	1.44	1.50
5	B	201	NAP	PN-O5D	4.10	1.75	1.59
5	B	201	NAP	C2N-N1N	3.59	1.39	1.35
5	B	201	NAP	C7N-N7N	3.54	1.39	1.33
5	A	205	NAP	O2B-C2B	-3.40	1.31	1.44
5	B	201	NAP	O2B-C2B	-3.14	1.32	1.44
5	B	201	NAP	O4B-C1B	2.83	1.45	1.41
5	B	201	NAP	C6N-C5N	-2.51	1.33	1.38
5	A	205	NAP	O4B-C4B	-2.40	1.39	1.45
5	A	205	NAP	C2N-N1N	2.39	1.37	1.35
5	A	205	NAP	C6N-C5N	-2.30	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	203	X0V	C6-N2	2.21	1.45	1.37
5	A	205	NAP	C2N-C3N	-2.20	1.35	1.39
3	A	203	X0V	C3-N1	2.12	1.44	1.37
5	B	201	NAP	C3N-C7N	-2.11	1.47	1.50
5	A	205	NAP	C4A-N3A	2.11	1.38	1.35
5	B	201	NAP	O4D-C1D	2.07	1.44	1.41
5	B	201	NAP	O2D-C2D	-2.04	1.38	1.43
5	A	205	NAP	C6N-N1N	2.03	1.40	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	205	NAP	C5N-C4N-C3N	-6.82	112.27	120.34
5	B	201	NAP	C5N-C4N-C3N	-6.79	112.31	120.34
5	B	201	NAP	PN-O3-PA	-5.42	114.22	132.83
5	A	205	NAP	PN-O3-PA	-5.28	114.70	132.83
5	A	205	NAP	O7N-C7N-C3N	4.20	124.66	119.63
5	A	205	NAP	C2N-C3N-C4N	3.95	122.74	118.26
5	B	201	NAP	O7N-C7N-C3N	3.64	123.99	119.63
5	A	205	NAP	O2B-P2B-O1X	-3.49	95.94	109.39
5	B	201	NAP	O2B-P2B-O1X	-3.37	96.37	109.39
5	B	201	NAP	C2N-C3N-C4N	3.22	121.91	118.26
5	B	201	NAP	O4D-C1D-C2D	-3.19	102.26	106.93
5	B	201	NAP	O7N-C7N-N7N	-2.85	118.52	122.58
5	A	205	NAP	PA-O5B-C5B	-2.77	105.42	121.68
5	B	201	NAP	PA-O5B-C5B	-2.77	105.45	121.68
3	A	203	X0V	C4-C3-C6	2.70	120.74	119.00
5	B	201	NAP	O3X-P2B-O2X	2.65	117.77	107.64
5	A	205	NAP	O3X-P2B-O2X	2.62	117.66	107.64
5	A	205	NAP	O7N-C7N-N7N	-2.58	118.91	122.58
5	B	201	NAP	PN-O5D-C5D	-2.51	106.97	121.68
5	B	201	NAP	C6N-C5N-C4N	2.50	123.07	119.44
5	B	201	NAP	C3B-C2B-C1B	-2.44	98.30	102.89
5	A	205	NAP	C2B-C3B-C4B	-2.29	97.01	101.99
5	A	205	NAP	O5D-PN-O1N	-2.27	100.18	109.07
5	A	205	NAP	C2A-N1A-C6A	-2.27	114.88	118.75
5	A	205	NAP	C6N-C5N-C4N	2.19	122.62	119.44
5	A	205	NAP	PN-O5D-C5D	-2.19	108.86	121.68
5	B	201	NAP	C2A-N1A-C6A	-2.16	115.06	118.75
5	B	201	NAP	C3D-C2D-C1D	-2.12	97.79	100.98
5	B	201	NAP	O5D-PN-O1N	-2.10	100.88	109.07
5	B	201	NAP	C6N-N1N-C2N	-2.08	120.08	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	205	NAP	O4D-C1D-C2D	-2.05	103.93	106.93
3	A	203	X0V	F1-C1-C2	-2.04	108.45	112.93
5	B	201	NAP	O3X-P2B-O2B	-2.03	96.89	105.99

There are no chirality outliers.

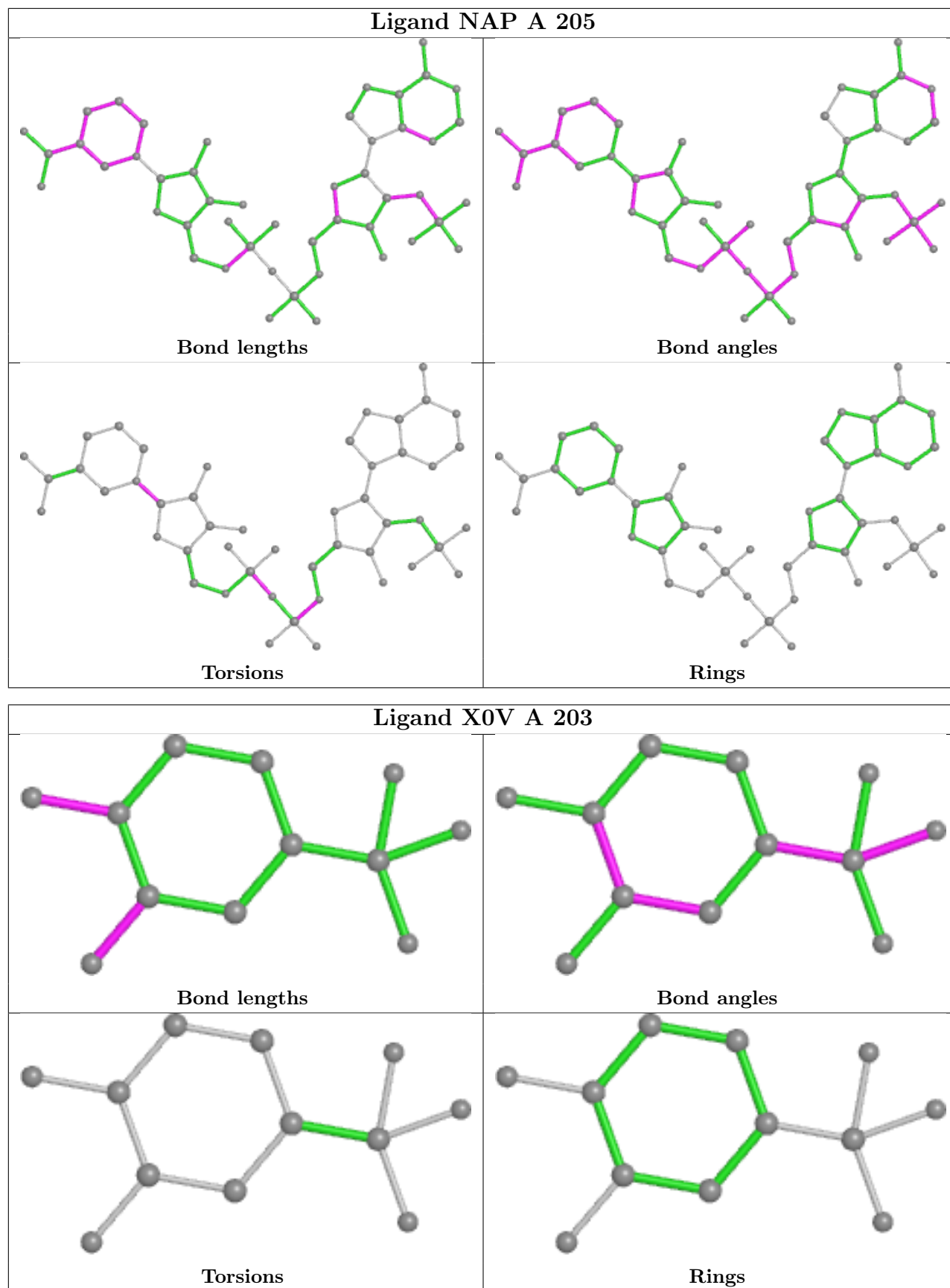
All (10) torsion outliers are listed below:

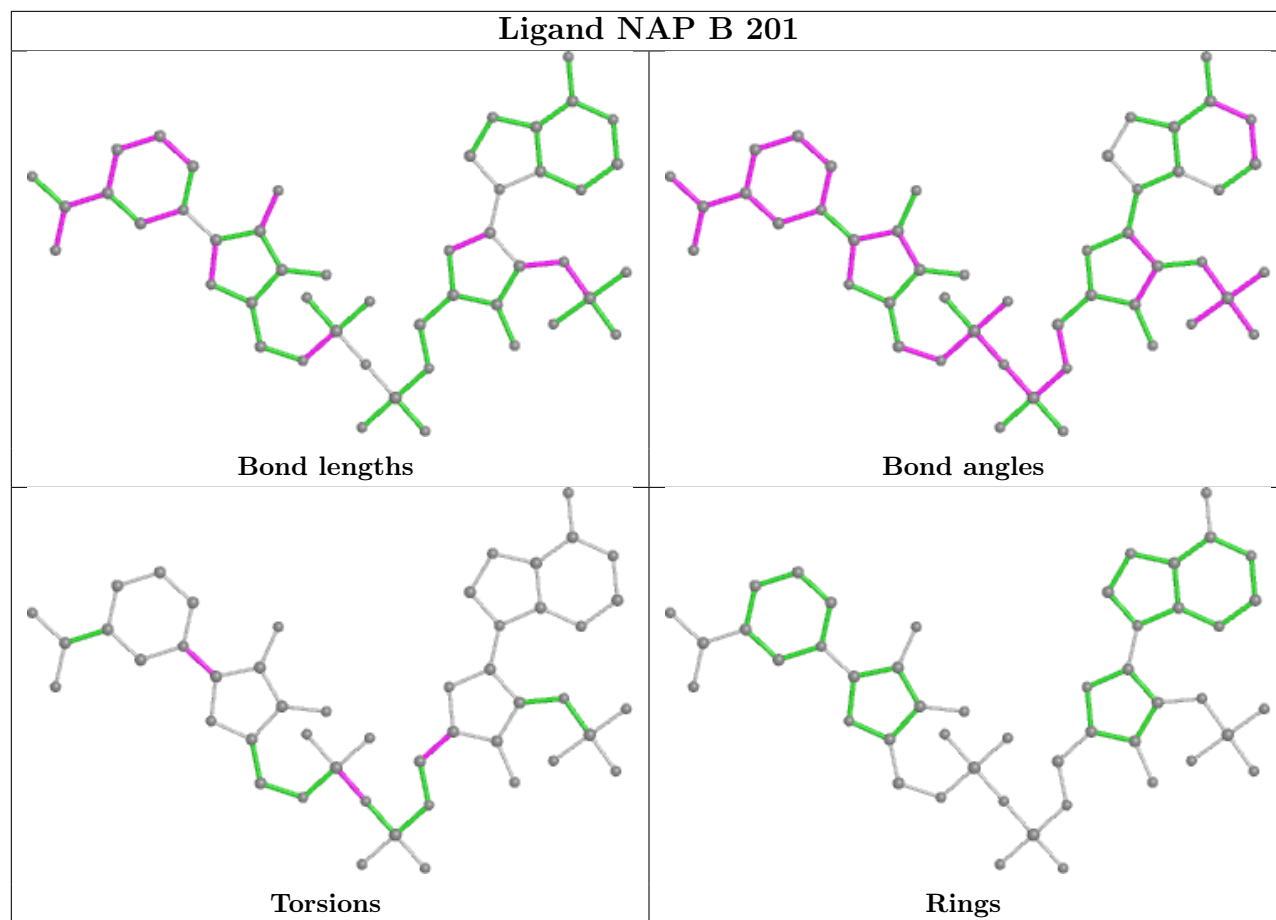
Mol	Chain	Res	Type	Atoms
5	A	205	NAP	C5B-O5B-PA-O1A
5	A	205	NAP	O4D-C1D-N1N-C6N
5	B	201	NAP	O4D-C1D-N1N-C2N
5	B	201	NAP	O4D-C1D-N1N-C6N
5	B	201	NAP	C2D-C1D-N1N-C2N
5	A	205	NAP	PA-O3-PN-O5D
5	B	201	NAP	PA-O3-PN-O5D
5	A	205	NAP	C5B-O5B-PA-O3
5	B	201	NAP	C3B-C4B-C5B-O5B
5	B	201	NAP	C2D-C1D-N1N-C6N

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.