



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2020 – 01:07 PM BST

PDB ID : 6ZVM  
Title : Botulinum neurotoxin B2 binding domain in complex with GD1a  
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Deposited on : 2020-07-25  
Resolution : 1.80 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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
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) : 2.14.6

## 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 1.80 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

There are 4 unique types of molecules in this entry. The entry contains 4075 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 Neurotoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	425	Total	C	N	O	S	0	9	0
			3677	2366	604	697	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	854	SER	-	expression tag	UNP Q8GR96
AAA	855	HIS	-	expression tag	UNP Q8GR96
AAA	856	MET	-	expression tag	UNP Q8GR96

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	6	Total	C	N	O	0	0	0
			88	48	3	37			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	296	Total	O	0	2
			298	298		

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, $\alpha$ , $\beta$ , $\gamma$	139.64Å 56.16Å 76.79Å 90.00° 122.00° 90.00°	Depositor
Resolution (Å)	63.73 – 1.80	Depositor
% Data completeness (in resolution range)	99.5 (63.73-1.80)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.164 , 0.203	Depositor
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.514	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h-2*k,l	Xtriage
Total number of atoms	4075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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](#)

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](#)

6 monosaccharides 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	BGC	A	1	2	12,12,12	0.45	0	17,17,17	0.58	0
2	GAL	A	2	2	11,11,12	0.30	0	15,15,17	1.66	2 (13%)
2	NGA	A	3	2	14,14,15	0.68	0	17,19,21	1.16	2 (11%)
2	GAL	A	4	2	11,11,12	0.58	0	15,15,17	0.89	0
2	SIA	A	5	2	17,20,21	0.24	0	21,28,31	0.67	0
2	SIA	A	6	2	17,20,21	0.26	0	21,28,31	0.65	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	BGC	A	1	2	-	0/2/22/22	0/1/1/1
2	GAL	A	2	2	-	0/2/19/22	0/1/1/1
2	NGA	A	3	2	-	1/6/23/26	0/1/1/1
2	GAL	A	4	2	-	0/2/19/22	0/1/1/1
2	SIA	A	5	2	-	2/14/34/38	0/1/1/1
2	SIA	A	6	2	-	2/14/34/38	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	GAL	O3-C3-C2	-4.65	101.09	109.99
2	A	3	NGA	O3-C3-C4	2.80	116.83	110.35
2	A	3	NGA	O3-C3-C2	-2.61	104.07	109.47
2	A	2	GAL	C1-C2-C3	2.47	112.70	109.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6	SIA	C11-C10-N5-C5
2	A	6	SIA	O10-C10-N5-C5
2	A	5	SIA	C11-C10-N5-C5
2	A	5	SIA	O10-C10-N5-C5
2	A	3	NGA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 4.6 Ligand geometry

2 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	GOL	AAA	1302	-	5,5,5	0.08	0	5,5,5	0.23	0
3	GOL	AAA	1301	-	5,5,5	0.19	0	5,5,5	0.62	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
3	GOL	AAA	1302	-	-	3/4/4/4	-
3	GOL	AAA	1301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	1301	GOL	C1-C2-C3-O3
3	AAA	1301	GOL	O2-C2-C3-O3
3	AAA	1302	GOL	C1-C2-C3-O3
3	AAA	1302	GOL	O1-C1-C2-O2
3	AAA	1302	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.



## 4.7 Other polymers

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 ⓘ

### 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.