



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:14 AM EDT

PDB ID : 6MCX  
Title : INFLUENZA VIRUS NEURAMINIDASE SUBTYPE N9 (TERN) RECOMBINANT HEAD DOMAIN  
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Deposited on : 2018-09-02  
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**  
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 3590 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.

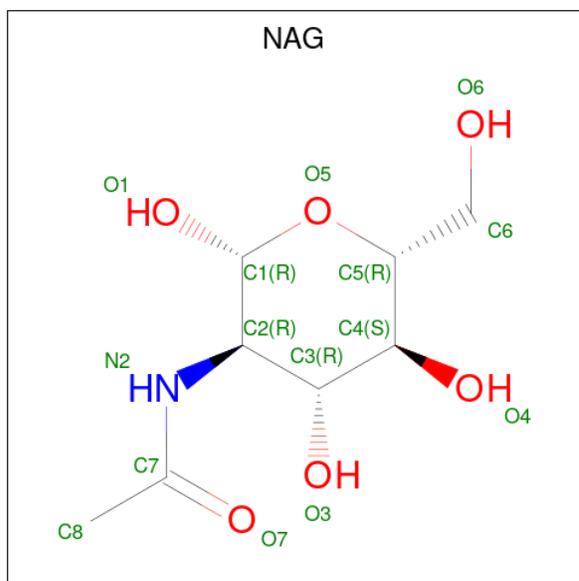
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3095	1925	546	601	23	0	11	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	7	83	46	2	35	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

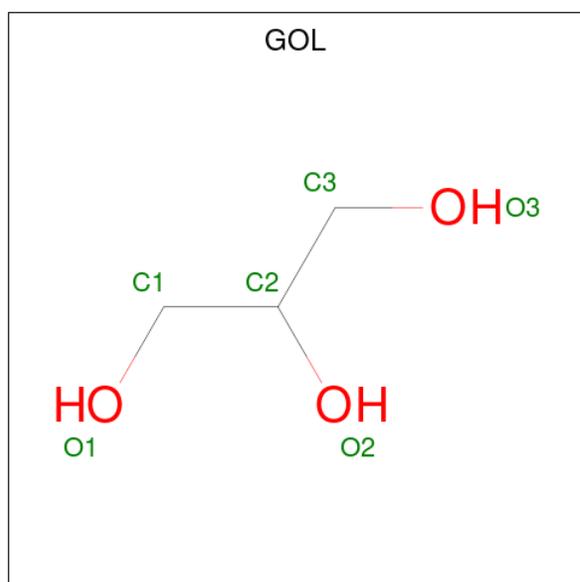


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 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
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	365	Total	O	0	0
			365	365		

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	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.72Å 180.72Å 180.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.22 – 2.30	Depositor
% Data completeness (in resolution range)	98.1 (45.22-2.30)	Depositor
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.147 , 0.206	Depositor
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtrriage
Anisotropy	0.000	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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](#)

7 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	NAG	B	1	1,2	14,14,15	0.70	0	17,19,21	2.18	5 (29%)
2	NAG	B	2	2	14,14,15	0.52	0	17,19,21	1.23	2 (11%)
2	BMA	B	3	2	11,11,12	0.44	0	15,15,17	1.46	2 (13%)
2	MAN	B	4	2	11,11,12	0.57	0	15,15,17	2.23	5 (33%)
2	MAN	B	5	2	11,11,12	0.58	0	15,15,17	1.20	2 (13%)
2	MAN	B	6	2	11,11,12	0.80	0	15,15,17	1.00	1 (6%)
2	MAN	B	7	2	11,11,12	0.80	0	15,15,17	3.49	8 (53%)

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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	MAN	C1-O5-C5	10.90	126.96	112.19
2	B	1	NAG	C1-O5-C5	5.26	119.31	112.19
2	B	4	MAN	C1-O5-C5	5.02	119.00	112.19
2	B	4	MAN	O2-C2-C1	-4.45	100.05	109.15
2	B	1	NAG	C8-C7-N2	-3.94	109.43	116.10
2	B	1	NAG	C1-C2-N2	-3.71	104.15	110.49
2	B	7	MAN	C3-C4-C5	3.35	116.22	110.24
2	B	7	MAN	O4-C4-C5	-3.26	101.20	109.30
2	B	3	BMA	O5-C5-C6	3.17	112.17	107.20
2	B	7	MAN	O5-C1-C2	2.98	115.37	110.77
2	B	7	MAN	C1-C2-C3	-2.97	106.02	109.67
2	B	4	MAN	O4-C4-C3	2.95	117.17	110.35
2	B	1	NAG	O7-C7-C8	2.92	127.47	122.06
2	B	4	MAN	O6-C6-C5	-2.78	101.77	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	MAN	O2-C2-C3	2.68	115.51	110.14
2	B	4	MAN	C6-C5-C4	-2.67	106.74	113.00
2	B	7	MAN	O6-C6-C5	2.62	120.29	111.29
2	B	3	BMA	C6-C5-C4	-2.55	107.04	113.00
2	B	5	MAN	O4-C4-C3	-2.48	104.62	110.35
2	B	2	NAG	C1-C2-N2	2.36	114.53	110.49
2	B	7	MAN	O3-C3-C4	2.36	115.81	110.35
2	B	2	NAG	C8-C7-N2	2.25	119.90	116.10
2	B	1	NAG	C2-N2-C7	-2.23	119.72	122.90
2	B	6	MAN	O5-C5-C6	2.19	110.64	107.20
2	B	5	MAN	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

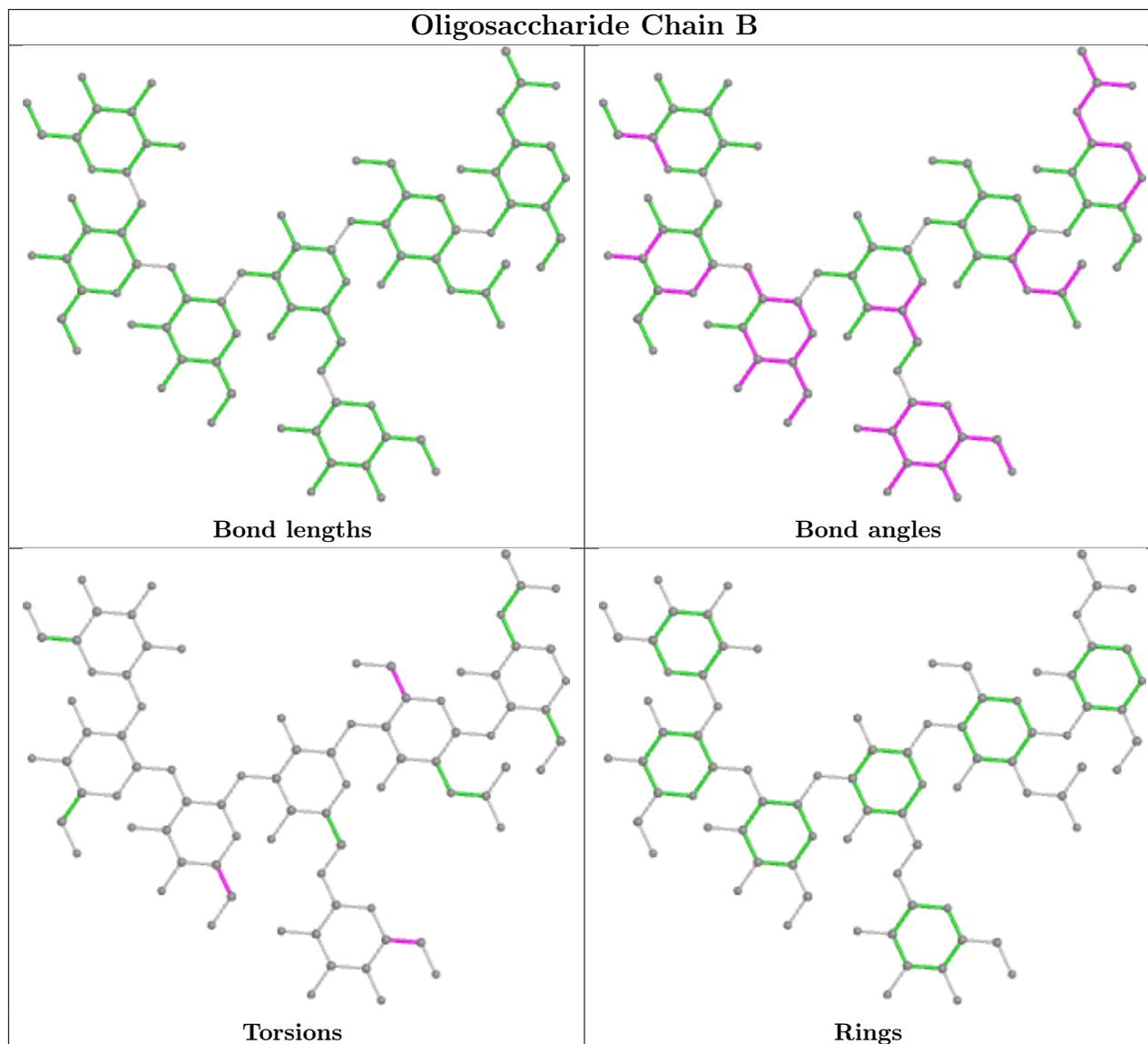
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C4-C5-C6-O6
2	B	7	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6

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 oligosaccharide.



## 4.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	GOL	A	511	-	5,5,5	0.12	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	508	1	14,14,15	0.75	0	17,19,21	1.49	5 (29%)
5	GOL	A	513	-	5,5,5	0.14	0	5,5,5	0.38	0
5	GOL	A	512	-	5,5,5	0.44	0	5,5,5	1.05	0
3	NAG	A	509	1	14,14,15	0.42	0	17,19,21	1.55	2 (11%)

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	GOL	A	511	-	-	0/4/4/4	-
3	NAG	A	508	1	-	0/6/23/26	0/1/1/1
5	GOL	A	513	-	-	4/4/4/4	-
5	GOL	A	512	-	-	2/4/4/4	-
3	NAG	A	509	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	509	NAG	C4-C3-C2	3.42	116.03	111.02
3	A	509	NAG	C1-O5-C5	2.51	115.59	112.19
3	A	508	NAG	C6-C5-C4	2.49	118.84	113.00
3	A	508	NAG	C2-N2-C7	2.33	126.23	122.90
3	A	508	NAG	O5-C5-C4	-2.09	105.73	110.83
3	A	508	NAG	C1-C2-N2	2.08	114.05	110.49
3	A	508	NAG	O5-C5-C6	2.08	110.46	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	513	GOL	O1-C1-C2-C3
5	A	513	GOL	C1-C2-C3-O3
5	A	513	GOL	O2-C2-C3-O3
5	A	513	GOL	O1-C1-C2-O2
3	A	509	NAG	O5-C5-C6-O6
5	A	512	GOL	O1-C1-C2-O2
5	A	512	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.