

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 2, 2023 – 04:28 PM EDT

PDB ID : 6NSC

Title: Crystal structure of the A/Brisbane/10/2007 (H3N2) influenza virus hemag-

glutinin G186V/L194P mutant apo form

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Deposited on : 2019-01-24

Resolution : 2.25 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 (i) 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 (i)) 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) : 2.35.1

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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 7 unique types of molecules in this entry. The entry contains 4321 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	317	Total	С	N	О	S	0	3	0
1	Λ	317	2489	1561	441	475	12		9	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP A8W893
A	10	GLY	-	expression tag	UNP A8W893
A	186	VAL	GLY	engineered mutation	UNP A8W893
A	194	PRO	LEU	engineered mutation	UNP A8W893

• Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	173	Total 1409	C 881	N 245	O 277	S 6	0	3	0

• Molecule 3 is an oligosaccharide called 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
3	С	5	Total 61	C 34		0	0	0

• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[be ta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

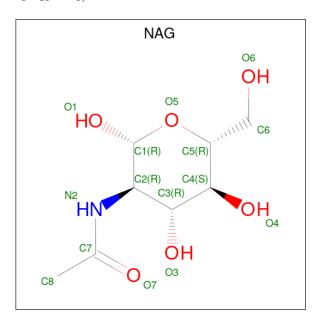
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total 38	C 22	N 2	O 14	0	0	0



 $\bullet$  Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total 28	16	2	10	0	0	0
5	F	2	Total 28	C 16			0	0	0

 $\bullet$  Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $\rm C_8H_{15}NO_6).$ 



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

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	121	Total O 121 121	0	0
7	В	119	Total O 119 119	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	H 3 2	Depositor	
Cell constants	100.60Å 100.60Å 384.46Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	50.00 - 2.25	Depositor	
% Data completeness	99.8 (50.00-2.25)	Depositor	
(in resolution range)	,	-	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	0.10	Depositor	
$< I/\sigma(I) > 1$	2.67  (at  2.24Å)	Xtriage	
Refinement program	REFMAC 5.8.0158	Depositor	
$R, R_{free}$	0.198 , 0.228	Depositor	
Wilson B-factor $(\mathring{A}^2)$	40.1	Xtriage	
Anisotropy	0.204	Xtriage	
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4321	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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)

12 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	Trino	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	С	1	1,3	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
3	NAG	С	2	3	14,14,15	0.43	0	17,19,21	0.89	1 (5%)
3	BMA	С	3	3	11,11,12	0.38	0	15,15,17	0.90	1 (6%)
3	MAN	С	4	3	11,11,12	0.49	0	15,15,17	1.21	2 (13%)
3	MAN	С	5	3	11,11,12	0.67	0	15,15,17	1.63	2 (13%)
4	NAG	D	1	4,1	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
4	NAG	D	2	4	14,14,15	0.36	0	17,19,21	1.15	1 (5%)
4	FUL	D	3	4	10,10,11	0.42	0	14,14,16	1.01	1 (7%)
5	NAG	Е	1	1,5	14,14,15	0.63	0	17,19,21	1.21	1 (5%)
5	NAG	Е	2	5	14,14,15	0.69	0	17,19,21	1.58	4 (23%)
5	NAG	F	1	1,5	14,14,15	0.46	0	17,19,21	0.84	0
5	NAG	F	2	5	14,14,15	0.37	0	17,19,21	0.63	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	NAG	С	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	0/6/23/26	0/1/1/1
3	BMA	С	3	3	-	2/2/19/22	0/1/1/1
3	MAN	С	4	3	-	2/2/19/22	0/1/1/1
3	MAN	С	5	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	FUL	D	3	4	-	-	0/1/1/1
5	NAG	Е	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	_	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	С	5	MAN	C1-O5-C5	4.23	117.93	112.19
5	Е	1	NAG	C1-O5-C5	4.16	117.82	112.19
3	С	5	MAN	C1-C2-C3	3.92	114.49	109.67

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	С	1	NAG	C1-O5-C5	3.75	117.27	112.19
4	D	2	NAG	C4-C3-C2	3.21	115.72	111.02
3	С	4	MAN	C3-C4-C5	3.03	115.64	110.24
5	Е	2	NAG	C1-O5-C5	3.00	116.26	112.19
5	Ε	2	NAG	O5-C5-C6	2.76	111.53	107.20
5	Е	2	NAG	C4-C3-C2	2.40	114.53	111.02
3	С	2	NAG	C1-O5-C5	2.32	115.34	112.19
4	D	3	FUL	O5-C1-C2	-2.26	107.28	110.77
3	С	4	MAN	C1-O5-C5	2.26	115.25	112.19
5	Ε	2	NAG	O5-C5-C4	-2.16	105.56	110.83
3	С	3	BMA	O5-C5-C6	2.03	110.38	107.20
4	D	1	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

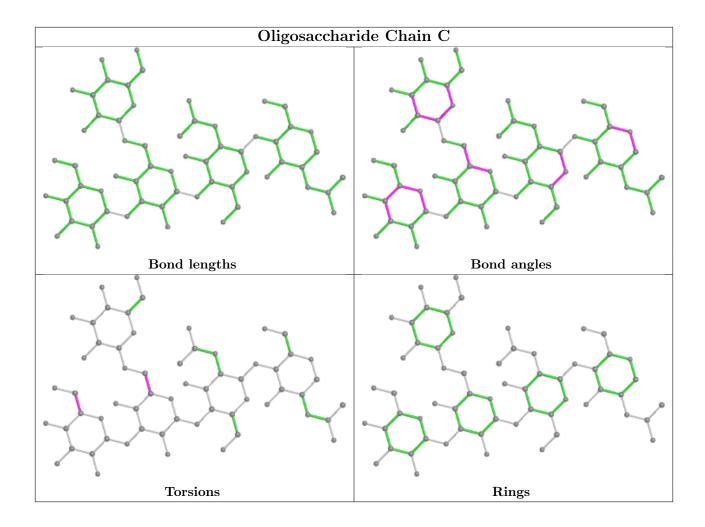
Mol	Chain	Res	Type	Atoms	
3	С	3	BMA	C4-C5-C6-O6	
3	С	3	BMA	O5-C5-C6-O6	
3	С	4	MAN	O5-C5-C6-O6	
5	Е	2	NAG	O5-C5-C6-O6	
3	С	4	MAN	C4-C5-C6-O6	
5	Е	2	NAG	C4-C5-C6-O6	
5	F	2	NAG	C4-C5-C6-O6	
5	F	2	NAG	O5-C5-C6-O6	

There are no ring outliers.

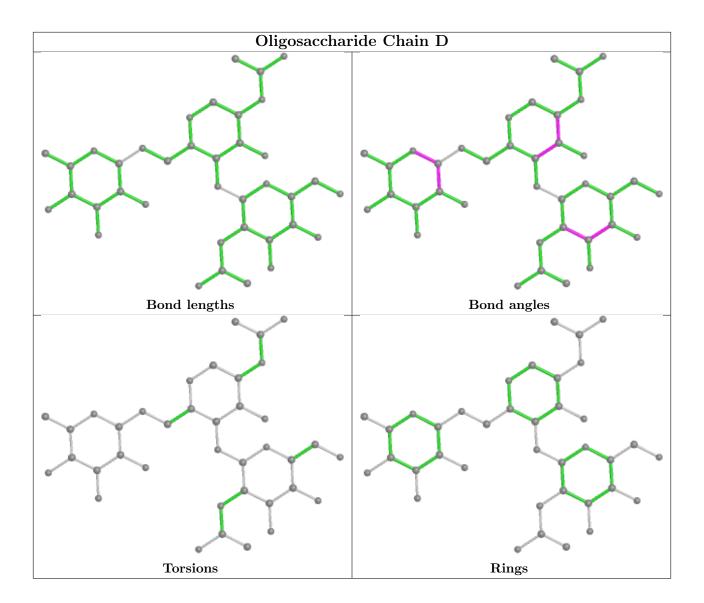
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

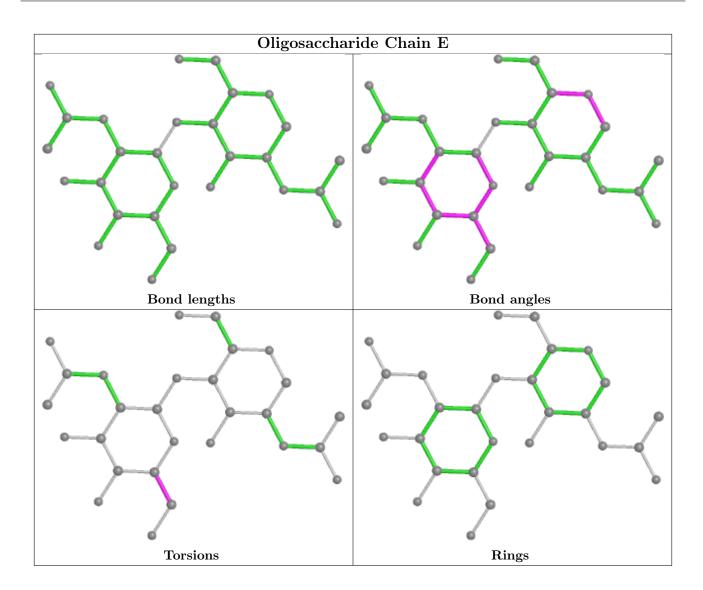




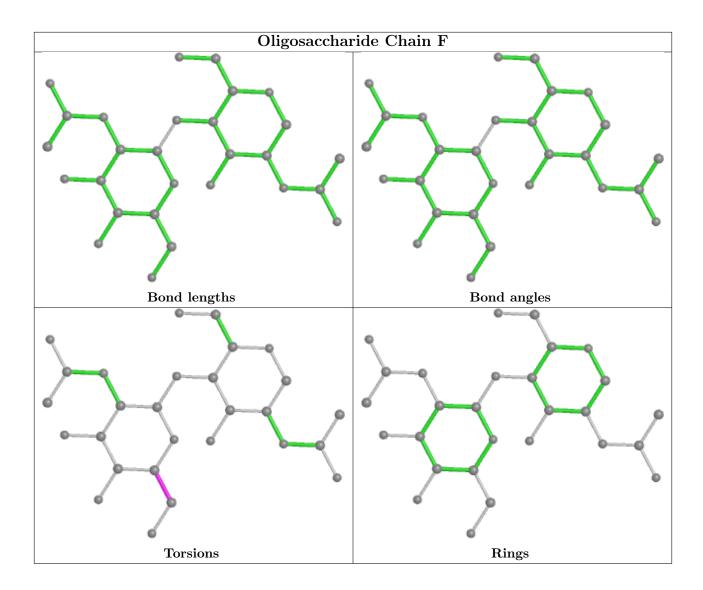












### 4.6 Ligand geometry (i)

#### 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		
IVIOI	Туре				Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	414	1	14,14,15	0.50	0	17,19,21	0.87	0
6	NAG	A	401	1	14,14,15	0.64	0	17,19,21	1.53	1 (5%)



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
6	NAG	A	414	1	-	0/6/23/26	0/1/1/1
6	NAG	A	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
6	A	401	NAG	C1-O5-C5	5.20	119.24	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 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.

