

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

#### Oct 2, 2023 – 02:06 PM EDT

PDB ID : 6NSG

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

glutinin G186V/L194P mutant in complex with 6'-SLNLN

Authors: Wu, N.C.; Wilson, I.A.

Deposited on : 2019-01-24

Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

MolProbity : FAILED

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (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 (i)

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 8 unique types of molecules in this entry. The entry contains 4287 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		$\mathbf{At}$	oms			ZeroOcc	AltConf	Trace
1	A	317	Total 2484	C 1559	N 441	O 472	S 12	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP C3PR70
A	10	GLY	-	expression tag	UNP C3PR70
A	190	ASP	ASN	conflict	UNP C3PR70
A	194	PRO	LEU	engineered mutation	UNP C3PR70

• Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	173	Total 1413	C 885	N 245	O 277	S 6	0	4	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	A	Aton	ns	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.

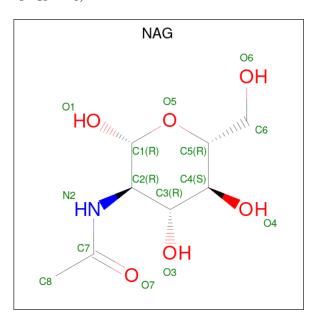
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total 38	C 22	N 2	O 14	0	0	0



 $\bullet$  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 C N O 28 16 2 10	0	0	0
5	F	2	Total C N O 28 16 2 10	0	0	0

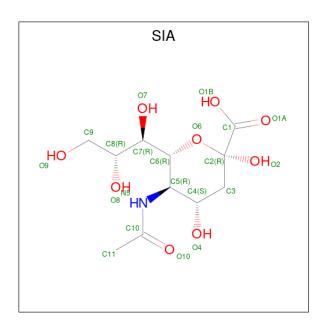
• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

• Molecule 7 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	Λ	1	Total	С	N	О	0	0
'	A	1	21	11	1	9	U	0

### • Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	84	Total O 84 84	0	0
8	В	88	Total O 88 88	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	100.26Å 100.26Å 383.64Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	50.00 - 2.40	Depositor	
% Data completeness	100.0 (50.00-2.40)	Depositor	
(in resolution range)	,	-	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	0.10	Depositor	
$< I/\sigma(I) > 1$	2.94  (at  2.39Å)	Xtriage	
Refinement program	REFMAC 5.8.0158	Depositor	
$R, R_{free}$	0.187 , 0.231	Depositor	
Wilson B-factor $(A^2)$	48.2	Xtriage	
Anisotropy	0.154	Xtriage	
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4287	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.47% 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	Tuna	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	С	1	1,3	14,14,15	0.53	0	17,19,21	1.36	1 (5%)
3	NAG	С	2	3	14,14,15	0.42	0	17,19,21	1.13	1 (5%)
3	BMA	С	3	3	11,11,12	0.40	0	15,15,17	0.82	0
3	MAN	С	4	3	11,11,12	0.44	0	15,15,17	1.13	2 (13%)
3	MAN	С	5	3	11,11,12	0.75	0	15,15,17	2.36	3 (20%)
4	NAG	D	1	1,4	14,14,15	0.50	0	17,19,21	1.28	3 (17%)
4	NAG	D	2	4	14,14,15	0.36	0	17,19,21	0.83	1 (5%)
4	FUL	D	3	4	10,10,11	0.47	0	14,14,16	0.79	0
5	NAG	Е	1	1,5	14,14,15	0.51	0	17,19,21	1.25	1 (5%)
5	NAG	Е	2	5	14,14,15	0.51	0	17,19,21	1.40	1 (5%)
5	NAG	F	1	1,5	14,14,15	0.44	0	17,19,21	0.90	1 (5%)
5	NAG	F	2	5	14,14,15	0.29	0	17,19,21	0.44	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	-	2/6/23/26	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	FUL	D	3	4	-	-	0/1/1/1
5	NAG	Ε	1	1,5	1	0/6/23/26	0/1/1/1
5	NAG	Ε	2	5	-	0/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mathbf{Ideal}(^o)$
3	С	5	MAN	C1-C2-C3	6.50	117.66	109.67
3	С	5	MAN	C1-O5-C5	4.65	118.49	112.19
5	Ε	2	NAG	C1-O5-C5	4.63	118.46	112.19

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
3	С	1	NAG	C1-O5-C5	4.33	118.06	112.19
5	Е	1	NAG	C1-O5-C5	3.98	117.59	112.19

There are no chirality outliers.

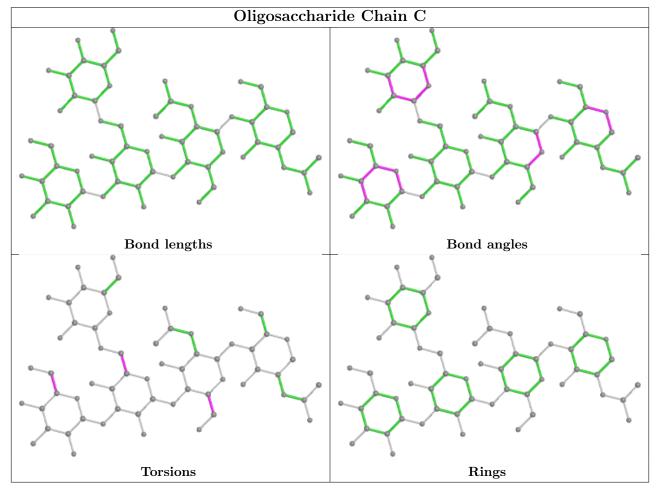
5 of 8 torsion outliers are listed below:

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

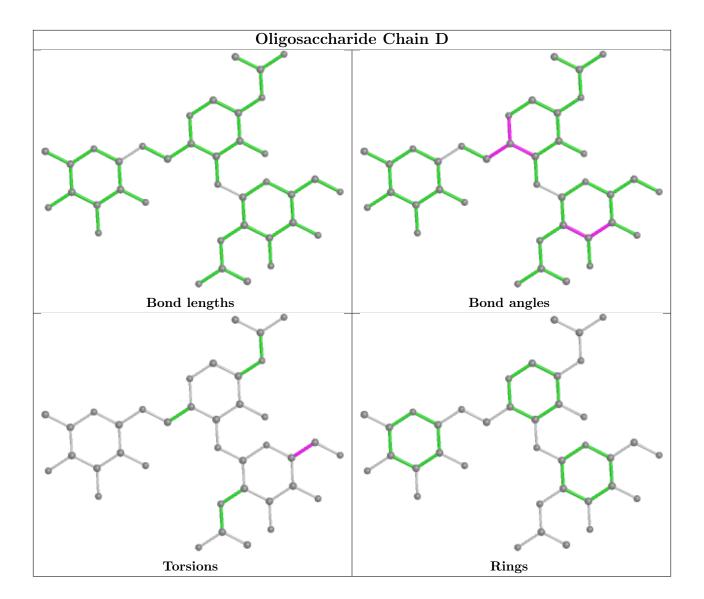
There are no ring outliers.

No monomer is involved in short contacts.

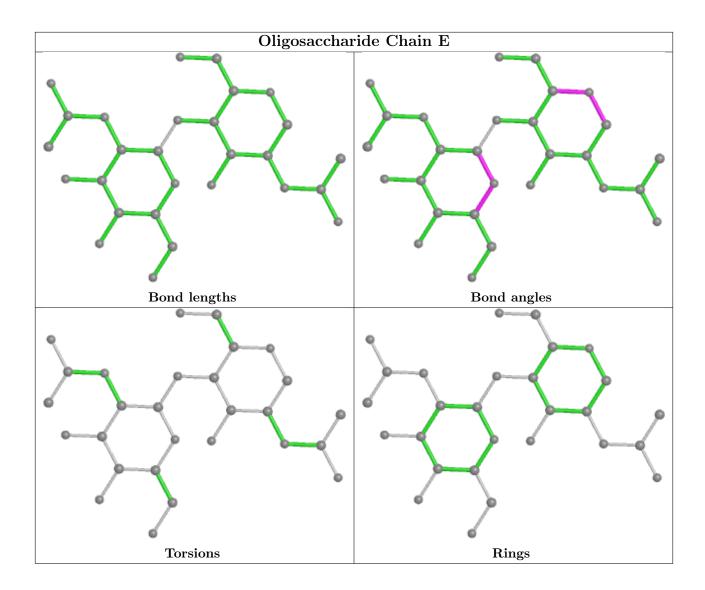
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



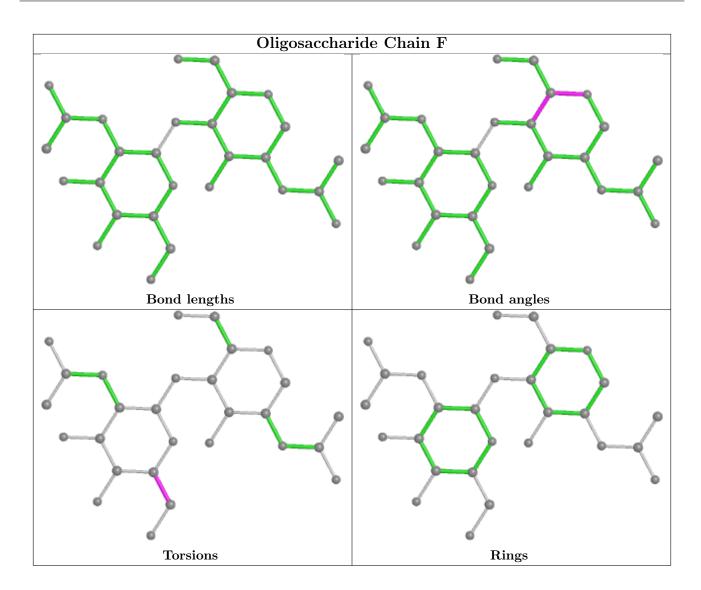












# 4.6 Ligand geometry (i)

#### 4 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	Trunc	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	Bo	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2								
6	NAG	A	414	1	14,14,15	0.53	0	17,19,21	0.99	1 (5%)								
6	NAG	В	201	2	14,14,15	0.46	0	17,19,21	1.03	1 (5%)								
7	SIA	A	415	-	21,21,21	0.97	1 (4%)	25,31,31	0.94	1 (4%)								



	Mol	Type	Chain	Res	Link	Bo	nd leng	ths	В	ond ang	les
	IVIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
Ī	6	NAG	A	401	1	14,14,15	0.58	0	17,19,21	1.16	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	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
6	NAG	A	414	1	-	0/6/23/26	0/1/1/1
6	NAG	В	201	2	-	0/6/23/26	0/1/1/1
7	SIA	A	415	-	-	3/20/38/38	0/1/1/1
6	NAG	A	401	1	-	0/6/23/26	0/1/1/1

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
7	A	415	SIA	O2-C2	3.27	1.43	1.39

#### All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
7	A	415	SIA	O1A-C1-C2	-3.00	119.05	123.59
6	A	401	NAG	C1-O5-C5	2.97	116.22	112.19
6	A	414	NAG	C1-O5-C5	2.59	115.70	112.19
6	A	401	NAG	O5-C5-C6	2.44	111.02	107.20
6	В	201	NAG	O5-C5-C6	2.26	110.75	107.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	415	SIA	C7-C8-C9-O9
7	A	415	SIA	O1A-C1-C2-O2
7	A	415	SIA	O8-C8-C9-O9

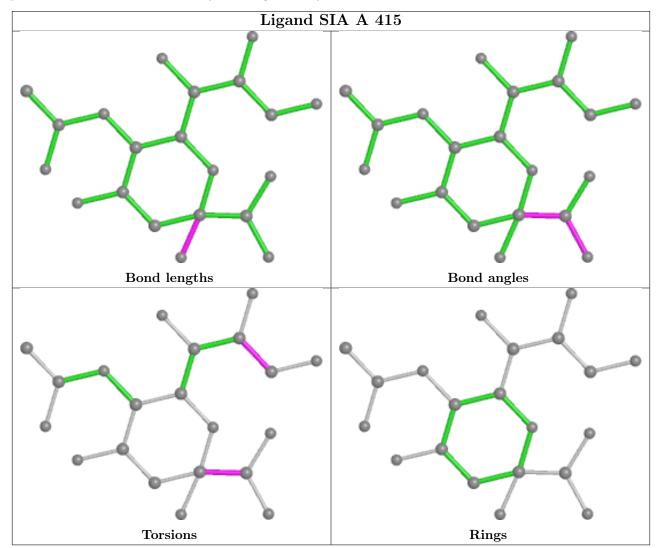
There are no ring outliers.

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 then 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.

