

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

Aug 9, 2020 – 05:19 AM BST

PDB ID : 1IVB

Title : STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS

NEURAMINIDASE

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Deposited on : 1994-12-12

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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

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

Xtriage (Phenix) : 1.13 EDS : 2.13.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

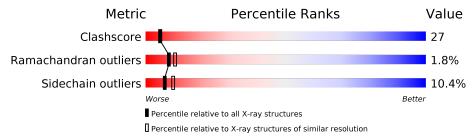
Validation Pipeline (wwPDB-VP) : 2.13.1

# 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.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality (	of chain	
1	Δ	390	53%	39%	7% •



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3785 atoms, of which 712 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.

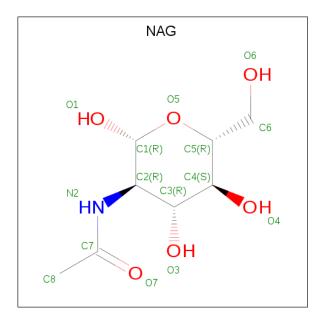
• Molecule 1 is a protein called INFLUENZA VIRUS B/LEE/40 NEURAMINIDASE.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total 3736	C 1907	H 696	N 531	O 574	S 28	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ARG	LYS	conflict	UNP P03474

• Molecule 2 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>).



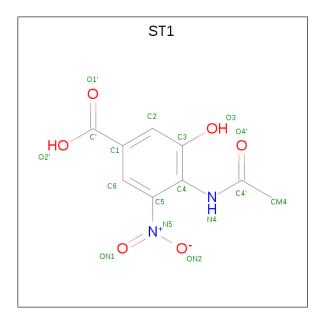
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	С	H	N	Ō	0	0
			28	8	14	1	Ъ		

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0

• Molecule 4 is 4-(ACETYLAMINO)-3-HYDROXY-5-NITROBENZOIC ACID (three-letter code: ST1) (formula:  $C_9H_8N_2O_6$ ).



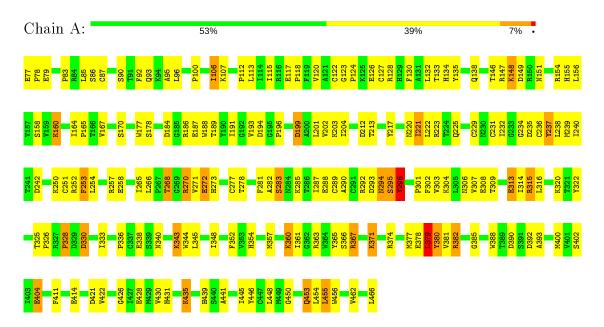
Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	
4	Λ	1	Total	С	Н	N	О	0	0
4	A	1	19	9	2	2	6	U	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: INFLUENZA VIRUS B/LEE/40 NEURAMINIDASE





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants	124.54Å 124.54Å 71.82Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 - 2.40	Depositor
Resolution (A)	23.52 - 2.42	EDS
% Data completeness	(Not available) (6.50-2.40)	Depositor
(in resolution range)	68.8 (23.52-2.42)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.56 (at 2.41Å)	Xtriage
Refinement program	X-PLOR	Depositor
P. P.	0.189 , (Not available)	Depositor
$R, R_{free}$	0.251 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.7	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38, 60.9	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.44, < L^2>=0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	3785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.72% 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.

# 5 Model quality (i)

#### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, ST1

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| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.74	0/3114	0.99	8/4210 (0.2%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	379	LEU	CA-CB-CG	9.92	138.12	115.30
1	A	290	ALA	N-CA-C	-6.36	93.83	111.00
1	A	296	TYR	N-CA-C	6.15	127.61	111.00
1	A	96	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	435	LYS	N-CA-C	5.24	125.14	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	TYR	Sidechain
1	A	365	TYR	Sidechain



#### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Α	3040	696	2934	159	0
2	A	14	14	13	2	0
3	A	2	0	0	0	0
4	A	17	2	7	0	0
All	All	3073	712	2954	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 160 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ ( ext{\AA}) \end{aligned}$
1:A:296:TYR:HA	1:A:343:LYS:HG3	1.42	1.01
1:A:270:ARG:HH11	1:A:270:ARG:HG3	1.39	0.86
1:A:268:THR:HG22	1:A:313:GLU:HG2	1.58	0.86
1:A:77:GLU:HB2	1:A:78:PRO:HD2	1.61	0.81
1:A:336:PRO:HB2	1:A:338:GLU:OE1	1.81	0.80

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	· ·				Percentiles
1	A	388/390 (100%)	346 (89%)	35 (9%)	7 (2%)	8 10

5 of 7 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	283	SER
1	A	296	TYR
1	A	345	LEU
1	A	392	ASP
1	A	328	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	326/326 (100%)	292 (90%)	34 (10%)	7 10		

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	THR
1	A	295	SER
1	A	453	GLN
1	A	272	GLU
1	A	160	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	220	ASN
1	A	439	HIS
1	A	294	ASN
1	A	134	HIS
1	A	340	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.



#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	467	1	14,14,15	3.26	3 (21%)	17,19,21	2.30	5 (29%)
4	ST1	A	471	-	14,17,17	2.43	2 (14%)	16,24,24	1.94	5 (31%)

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	${f Res}$	Link	Chirals	Torsions	Rings
2	NAG	A	467	1	-	1/6/23/26	0/1/1/1
4	ST1	A	471	-	-	4/6/12/12	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
2	A	467	NAG	O5-C1	9.94	1.59	1.43
4	A	471	ST1	C1-C'	-7.58	1.40	1.47
2	A	467	NAG	C4-C5	4.65	1.62	1.53
2	A	467	NAG	C4-C3	3.94	1.62	1.52
4	A	471	ST1	C5-N5	-3.59	1.39	1.45



The wors	t 5	of	10	bond	angle	outliers	are	listed	below:
		01		OILG	~115	OGGILOID	COLO	IIDCC	~ ~ ~ .

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
4	A	471	ST1	ON1-N5-C5	-4.75	110.90	119.03
2	A	467	NAG	O5-C1-C2	4.68	118.68	111.29
2	A	467	NAG	C2-N2-C7	-4.30	116.78	122.90
4	A	471	ST1	C4-N4-C4'	-4.17	115.75	122.79
2	A	467	NAG	C1-O5-C5	3.85	117.40	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	471	ST1	O4'-C4'-N4-C4
4	A	471	ST1	CM4-C4'-N4-C4
4	A	471	ST1	C4-C5-N5-ON1
4	A	471	ST1	C6-C5-N5-ON1
2	A	467	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
2	A	467	NAG	2	0

# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

#### 6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

