



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:35 PM GMT

PDB ID : 1NN2  
Title : THREE-DIMENSIONAL STRUCTURE OF THE NEURAMINIDASE OF INFLUENZA VIRUS A(SLASH)TOKYO(SLASH)3(SLASH)67AT 2.2 ANGSTROMS RESOLUTION  
Authors : Varghese, J.N.; Colman, P.M.  
Deposited on : 1991-03-28  
Resolution : 2.20 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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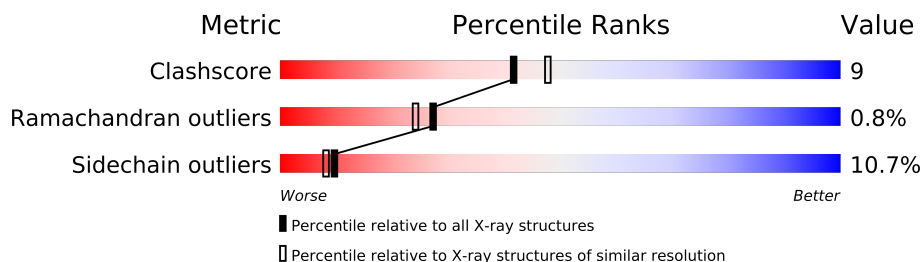
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	388	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4429 atoms, of which 1100 are hydrogens and 0 are deuterium.

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
1	A	388	Total	C	H	N	O	S	0	0	0
			3746	1866	724	545	588	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	H	N	O	28	0
			55	16	27	2	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	7	Total	C	H	N	O	S	69	0
			174	50	82	4	37	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820

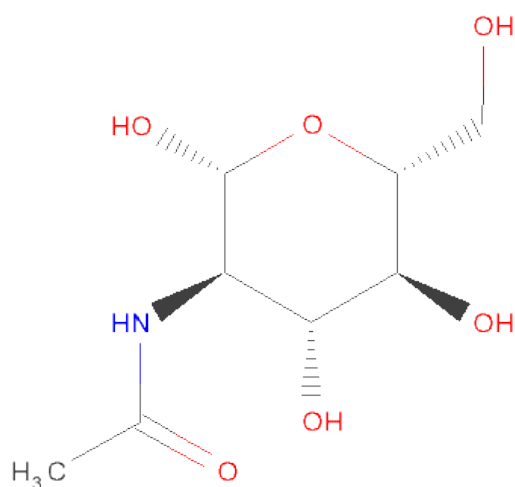
- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	6	Total	C	H	N	O	0	0
			139	40	67	2	30		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	CONFLICT	UNP P06820

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	28	0
			28	8	14	1	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is water.

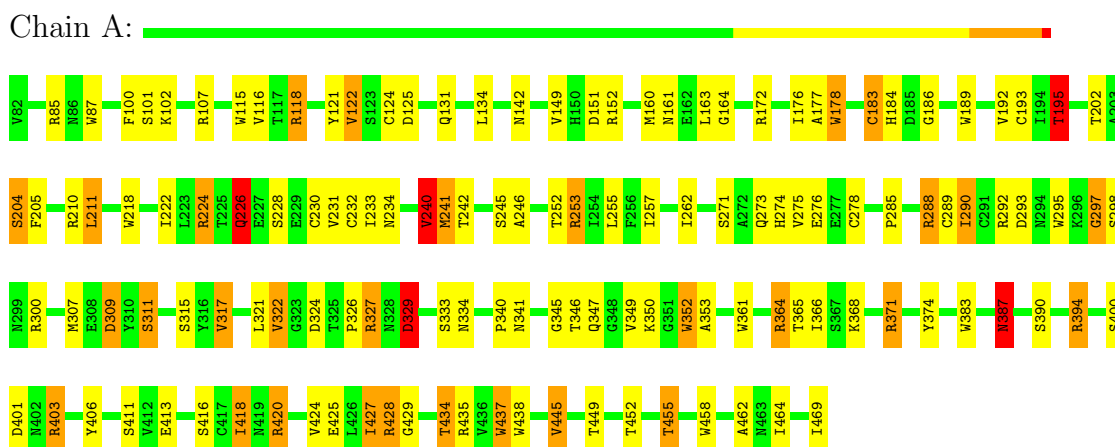
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	86	Total	H	O	0	0
			258	172	86		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

Note EDS failed to run properly.

#### • Molecule 1: NEURAMINIDASE



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.60Å 139.60Å 191.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.210 , (Not available)	Depositor
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.585	Xtriage
Estimated twinning fraction	0.043 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.047 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 30245 reflections	Xtriage
Total number of atoms	4429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, NGK, FUL, MAN

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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.99	3/3092 (0.1%)	1.91	104/4194 (2.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	VAL	CA-CB	5.83	1.67	1.54
1	A	122	VAL	CA-CB	5.56	1.66	1.54
1	A	231	VAL	CA-CB	5.20	1.65	1.54

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	A	124	CYS	N-CA-CB	-12.16	88.71	110.60
1	A	300	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	A	361	TRP	CD1-CG-CD2	10.44	114.66	106.30
1	A	224	ARG	NE-CZ-NH1	10.42	125.51	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3022	724	2135	52	0
2	A	28	27	0	0	0
3	A	92	82	0	0	0
4	A	72	67	0	0	0
5	A	28	28	0	4	0
6	A	1	0	0	0	0
7	A	86	172	0	3	0
All	All	3329	1100	2135	53	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 53 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:ILE:HG22	1:A:234:ASN:ND2	2.03	0.74
1:A:322:VAL:HG12	1:A:327:ARG:HG3	1.71	0.72
1:A:101:SER:HB3	1:A:445:VAL:HG13	1.77	0.67
1:A:226:GLN:HG3	1:A:278:CYS:O	1.95	0.67
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.76	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	386/388 (100%)	353 (92%)	30 (8%)	3 (1%)	27 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	222	ILE
1	A	322	VAL

### 5.3.2 Protein sidechains ⓘ

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	338/338 (100%)	302 (89%)	36 (11%)	10 8

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ILE
1	A	315	SER
1	A	452	THR
1	A	288	ARG
1	A	324	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	A	234	ASN
1	A	334	ASN
1	A	200	ASN
1	A	274	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

15 carbohydrates 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	A	470(A)	1,2	12,14,15	0.75	0	15,19,21	1.52	2 (13%)
2	NAG	A	471(B)	2	12,14,15	0.72	0	15,19,21	1.30	2 (13%)
3	NAG	A	472(A)	1,3	12,14,15	0.73	0	15,19,21	1.80	6 (40%)
3	NAG	A	473(B)	3	12,14,15	1.06	1 (8%)	15,19,21	1.21	1 (6%)
3	BMA	A	474(C)	3	10,11,12	1.02	0	11,15,17	1.30	2 (18%)
3	MAN	A	475(D)	3	10,11,12	0.88	0	11,15,17	1.07	1 (9%)
3	NAG	A	476(E)	3	12,14,15	1.07	2 (16%)	15,19,21	1.54	2 (13%)
3	NGK	A	477(F)	3	16,18,19	2.86	1 (6%)	22,26,28	1.95	5 (22%)
3	FUL	A	478(I)	3	9,10,11	3.35	3 (33%)	10,14,16	5.76	6 (60%)
4	NAG	A	479(A)	1,4	12,14,15	0.99	1 (8%)	15,19,21	1.17	2 (13%)
4	NAG	A	480(B)	4	12,14,15	0.89	0	15,19,21	2.13	5 (33%)
4	BMA	A	481(C)	4	10,11,12	0.70	0	11,15,17	1.28	2 (18%)
4	MAN	A	482(D)	4	10,11,12	0.64	0	11,15,17	1.34	1 (9%)
4	MAN	A	483(E)	4	10,11,12	0.57	0	11,15,17	0.95	0
4	MAN	A	484(F)	4	10,11,12	0.67	0	11,15,17	0.73	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	NAG	A	470(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	471(B)	2	-	0/6/23/26	0/1/1/1
3	NAG	A	472(A)	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	473(B)	3	-	0/6/23/26	0/1/1/1
3	BMA	A	474(C)	3	-	0/2/19/22	0/1/1/1
3	MAN	A	475(D)	3	-	0/2/19/22	0/1/1/1
3	NAG	A	476(E)	3	-	0/6/23/26	0/1/1/1
3	NGK	A	477(F)	3	-	0/11/28/31	0/1/1/1
3	FUL	A	478(I)	3	-	0/0/17/20	0/1/1/1
4	NAG	A	479(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	480(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	A	481(C)	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	482(D)	4	-	0/2/19/22	0/1/1/1
4	MAN	A	483(E)	4	-	0/2/19/22	0/1/1/1
4	MAN	A	484(F)	4	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	477(F)	NGK	O4-S	-11.09	1.42	1.60
3	A	478(I)	FUL	C4-C5	8.21	1.70	1.52
3	A	478(I)	FUL	C4-C3	4.74	1.65	1.52
3	A	478(I)	FUL	C6-C5	2.39	1.57	1.51
3	A	476(E)	NAG	C4-C5	2.38	1.58	1.53

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	478(I)	FUL	C6-C5-C4	11.68	132.03	113.06
3	A	478(I)	FUL	O3-C3-C2	11.34	130.67	109.94
3	A	477(F)	NGK	C8-C7-N	5.65	127.16	116.11
4	A	480(B)	NAG	C3-C2-N2	-4.59	104.78	111.76
3	A	478(I)	FUL	C3-C4-C5	4.42	117.21	109.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	485(A)	-	12,14,15	0.92	1 (8%)	15,19,21	1.40	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	486(B)	-	12,14,15	0.56	0	15,19,21	0.98	1 (6%)

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	NAG	A	485(A)	-	-	0/6/23/26	0/1/1/1
5	NAG	A	486(B)	-	-	0/6/23/26	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	485(A)	NAG	O5-C5	-2.39	1.41	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	485(A)	NAG	O5-C5-C4	-2.68	107.25	110.65
5	A	485(A)	NAG	C6-C5-C4	2.62	119.32	113.00
5	A	485(A)	NAG	C8-C7-N2	2.43	120.87	116.11
5	A	486(B)	NAG	O3-C3-C2	2.41	114.16	109.09
5	A	485(A)	NAG	O7-C7-C8	-2.07	118.00	122.04

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	486(B)	NAG	C1-C2-C3-C4-C5-O5

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.