



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 05:03 AM BST

PDB ID : 1NMA  
Title : N9 NEURAMINIDASE COMPLEXES WITH ANTIBODIES NC41 AND  
NC10: EMPIRICAL FREE-ENERGY CALCULATIONS CAPTURE SPECI-  
FICITY TRENDS OBSERVED WITH MUTANT BINDING DATA  
Authors : Tulip, W.R.; Varghese, J.N.; Colman, P.M.  
Deposited on : 1994-05-06  
Resolution : 3.00 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.13.1

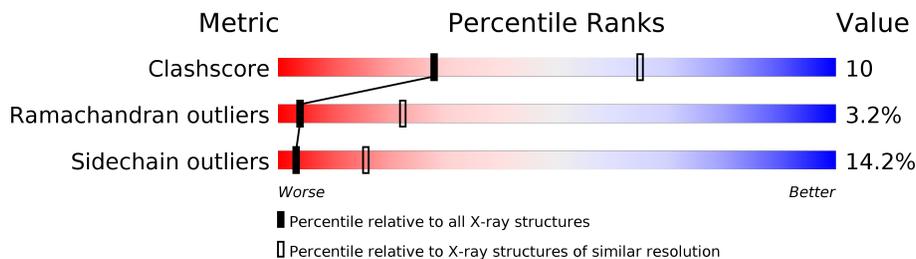
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	N	388	
2	L	109	
3	H	122	
4	A	6	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4863 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 N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	N	378	2979	1851	527	578	23	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	387	LYS	ARG	conflict	UNP P05803
N	389	ARG	LYS	conflict	UNP P05803

- Molecule 2 is a protein called FAB NC10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	109	853	530	142	178	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLN	GLU	conflict	GB 501094
L	4	MET	LEU	conflict	GB 501094

- Molecule 3 is a protein called FAB NC10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	122	945	594	154	192	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

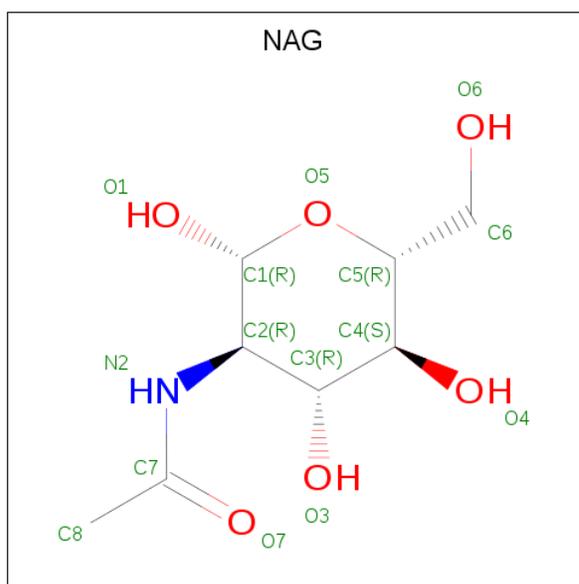
Chain	Residue	Modelled	Actual	Comment	Reference
H	7	PRO	SER	conflict	GB 501094
H	109	LEU	VAL	conflict	GB 501094

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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			
4	A	6	72	40	2	30	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



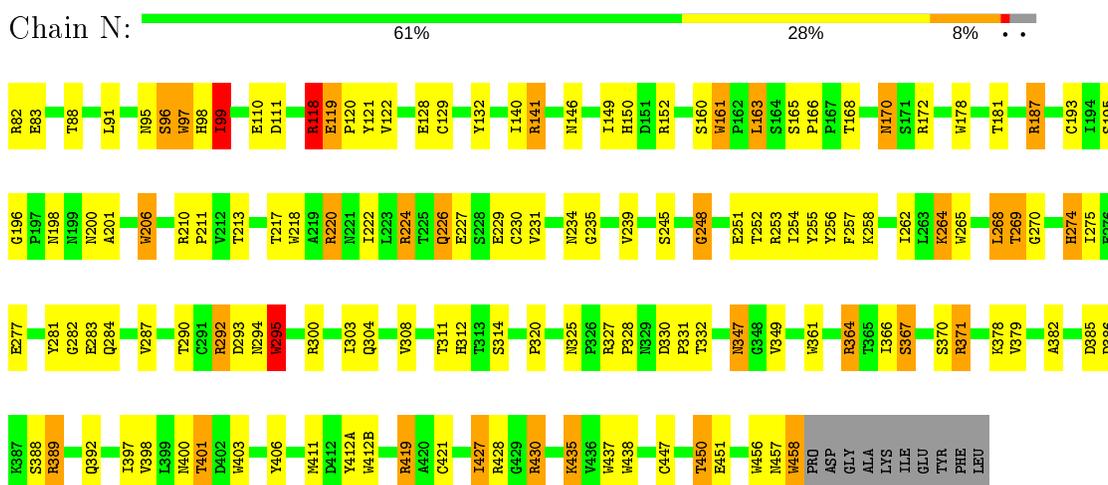
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	N	1	14	8	1	5	0	0

### 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.

Note EDS was not executed.

- Molecule 1: N9 NEURAMINIDASE



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

100%

  
MAG1  
MAG2  
EMAG3  
MAN4  
MAN5  
MAN6

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.50Å 171.50Å 160.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 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: BMA, NAG, 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	N	0.86	0/3058	1.81	88/4167 (2.1%)
2	L	0.81	1/869 (0.1%)	1.69	20/1178 (1.7%)
3	H	0.81	0/969	1.92	29/1311 (2.2%)
All	All	0.84	1/4896 (0.0%)	1.81	137/6656 (2.1%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	2
2	L	0	2
3	H	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	107	ARG	CZ-NH2	5.12	1.39	1.33

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	100	ARG	NE-CZ-NH1	18.95	129.78	120.30
3	H	100	ARG	NE-CZ-NH2	-17.86	111.37	120.30
1	N	364	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	N	265	TRP	CD1-CG-CD2	9.65	114.02	106.30
3	H	36	TRP	CD1-CG-CD2	9.53	113.92	106.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	90	TYR	Sidechain
2	L	107	ARG	Sidechain
2	L	108	ARG	Sidechain
1	N	248	GLY	Peptide
1	N	327	ARG	Peptide

## 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	N	2979	0	2800	53	0
2	L	853	0	810	20	0
3	H	945	0	882	18	0
4	A	72	0	61	0	0
5	N	14	0	13	0	0
All	All	4863	0	4566	90	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 10.

The worst 5 of 90 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:12:SER:HB2	2:L:107:ARG:HD3	1.48	0.95
3:H:3:GLN:HB2	3:H:25:SER:HB3	1.56	0.87
3:H:12:VAL:HG21	3:H:82(C):LEU:HD22	1.64	0.79
1:N:366:ILE:HD11	1:N:400:ASN:HB3	1.69	0.72
2:L:12:SER:CB	2:L:107:ARG:HD3	2.22	0.70

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	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	376/388 (97%)	326 (87%)	43 (11%)	7 (2%)	8	36
2	L	107/109 (98%)	85 (79%)	12 (11%)	10 (9%)	0	3
3	H	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	9	39
All	All	603/619 (97%)	521 (86%)	63 (10%)	19 (3%)	4	22

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	220	ARG
1	N	222	ILE
2	L	78	LEU
2	L	80	GLN
1	N	170	ASN

### 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	N	332/340 (98%)	290 (87%)	42 (13%)	4	19
2	L	97/97 (100%)	80 (82%)	17 (18%)	2	10
3	H	100/100 (100%)	84 (84%)	16 (16%)	2	12
All	All	529/537 (98%)	454 (86%)	75 (14%)	3	16

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	367	SER
1	N	457	ASN
3	H	95	SER
1	N	370	SER
1	N	427	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	216	ASN
1	N	234	ASN
1	N	347	ASN
1	N	198	ASN
1	N	346	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](#)

6 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$
4	NAG	A	1	1,4	14,14,15	1.71	4 (28%)	17,19,21	1.85	3 (17%)
4	NAG	A	2	4	14,14,15	1.36	2 (14%)	17,19,21	1.59	5 (29%)
4	BMA	A	3	4	11,11,12	0.92	0	15,15,17	1.00	1 (6%)
4	MAN	A	4	4	11,11,12	0.83	0	15,15,17	1.62	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	A	5	4	11,11,12	1.14	1 (9%)	15,15,17	1.63	3 (20%)
4	MAN	A	6	4	11,11,12	0.83	0	15,15,17	1.30	2 (13%)

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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	C1-C2	3.05	1.56	1.52
4	A	2	NAG	C4-C5	2.98	1.59	1.53
4	A	1	NAG	C3-C2	2.98	1.58	1.52
4	A	2	NAG	O5-C1	-2.91	1.39	1.43
4	A	1	NAG	O4-C4	2.28	1.48	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	C2-N2-C7	4.41	129.18	122.90
4	A	1	NAG	C1-C2-N2	-4.19	103.33	110.49
4	A	2	NAG	C4-C3-C2	-3.67	105.65	111.02
4	A	5	MAN	O3-C3-C2	3.23	116.18	109.99
4	A	5	MAN	C1-O5-C5	3.09	116.37	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C1-C2-N2-C7
4	A	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	5	MAN	C4-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
5	NAG	N	475(A)	1	14,14,15	0.97	1 (7%)	17,19,21	1.50	3 (17%)

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	N	475(A)	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	475(A)	NAG	C4-C5	-2.23	1.48	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	475(A)	NAG	C1-C2-N2	-3.02	105.33	110.49
5	N	475(A)	NAG	C8-C7-N2	2.57	120.45	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	N	475(A)	NAG	O5-C5-C6	2.47	111.08	107.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.