



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:07 PM GMT

PDB ID : 1NMA  
Title : N9 NEURAMINIDASE COMPLEXES WITH ANTIBODIES NC41 AND NC10: EMPIRICAL FREE-ENERGY CALCULATIONS CAPTURE SPECIFICITY TRENDS OBSERVED WITH MUTANT BINDING DATA  
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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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

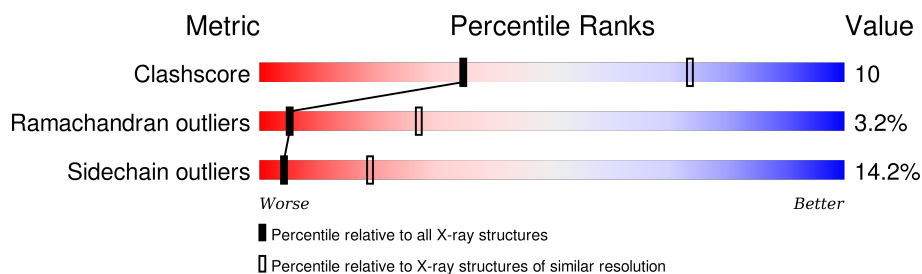
# 1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	N	388	 61% 28% 8% . .
2	L	109	 57% 31% 7% 5%
3	H	122	 57% 38% . .

## 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
1	N	378	Total	C	N	O	S	0	0	0
			2979	1851	527	578	23			

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
2	L	109	Total	C	N	O	S	0	0	0
			853	530	142	178	3			

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
3	H	122	Total	C	N	O	S	0	0	0
			945	594	154	192	5			

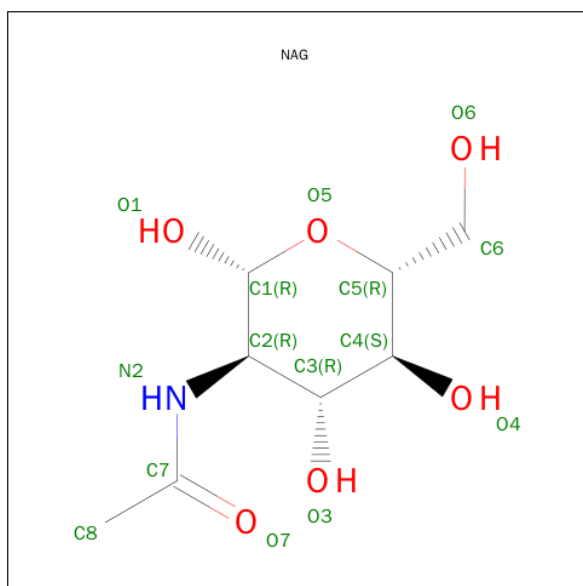
There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	N	6	Total	C	N	O	0	0
			72	40	2	30		

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



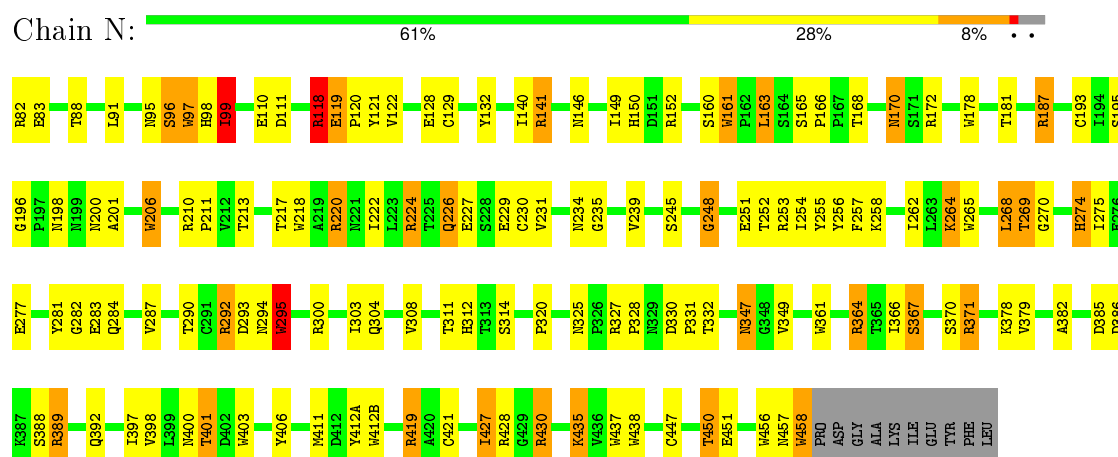
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	N	O	0	0
			14	8	1	5		

### 3 Residue-property plots

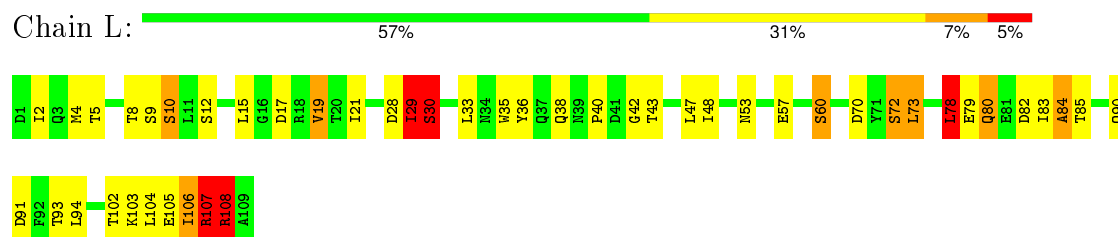
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 was not executed.

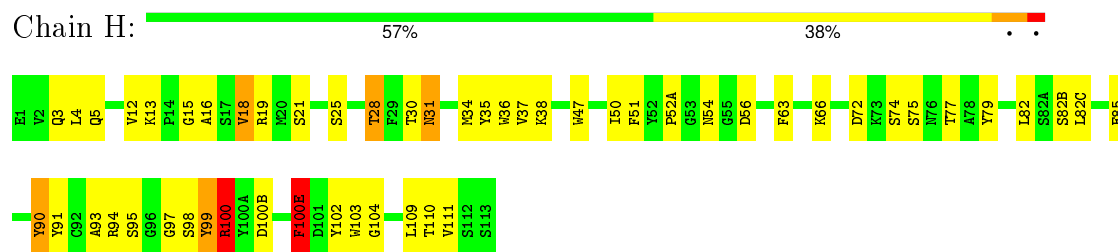
#### • Molecule 1: N9 NEURAMINIDASE



#### • Molecule 2: FAB NC10



#### • Molecule 3: FAB NC10



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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.	Xtriage
Total number of atoms	4863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 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, 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 ⓘ

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	N	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%)	10	43
2	L	107/109 (98%)	85 (79%)	12 (11%)	10 (9%)	1	4
3	H	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	11	46
All	All	603/619 (97%)	521 (86%)	63 (10%)	19 (3%)	5	27

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%)	5	23
2	L	97/97 (100%)	80 (82%)	17 (18%)	2	12
3	H	100/100 (100%)	84 (84%)	16 (16%)	3	15
All	All	529/537 (98%)	454 (86%)	75 (14%)	4	19

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 ⓘ

There are no RNA molecules 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 ⓘ

6 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$
4	NAG	N	469(A)	1,4	14,14,15	1.68	4 (28%)	15,19,21	1.61	2 (13%)
4	NAG	N	470(B)	4	14,14,15	1.32	2 (14%)	15,19,21	1.53	3 (20%)
4	BMA	N	471(C)	4	11,11,12	0.88	0	14,15,17	1.03	1 (7%)
4	MAN	N	472(D)	4	11,11,12	0.81	0	14,15,17	1.44	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	N	473(E)	4	11,11,12	1.14	1 (9%)	14,15,17	1.69	3 (21%)
4	MAN	N	474(F)	4	11,11,12	0.82	0	14,15,17	1.35	2 (14%)

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	N	469(A)	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	470(B)	4	-	0/6/23/26	0/1/1/1
4	BMA	N	471(C)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	472(D)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	473(E)	4	-	0/2/19/22	0/1/1/1
4	MAN	N	474(F)	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	N	470(B)	NAG	O5-C1	-2.78	1.39	1.43
4	N	473(E)	MAN	C2-C3	-2.36	1.49	1.52
4	N	469(A)	NAG	O4-C4	2.25	1.48	1.43
4	N	469(A)	NAG	C8-C7	2.32	1.55	1.50
4	N	469(A)	NAG	C3-C2	2.77	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	470(B)	NAG	C4-C3-C2	-3.59	105.65	111.23
4	N	474(F)	MAN	O4-C4-C3	-2.58	104.52	110.34
4	N	469(A)	NAG	O3-C3-C4	-2.53	104.65	110.34
4	N	473(E)	MAN	O4-C4-C3	-2.32	105.11	110.34
4	N	472(D)	MAN	C3-C4-C5	-2.07	106.58	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

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	0.96	1 (7%)	15,19,21	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
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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	475(A)	NAG	C2-N2-C7	-2.24	120.17	123.04
5	N	475(A)	NAG	C8-C7-N2	2.27	120.45	116.11

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

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.