



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 11:48 PM GMT

PDB ID : 1A14
Title : COMPLEX BETWEEN NC10 ANTI-INFLUENZA VIRUS NEURAMINIDASE SINGLE CHAIN ANTIBODY WITH A 5 RESIDUE LINKER AND INFLUENZA VIRUS NEURAMINIDASE
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Deposited on : 1997-12-21
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

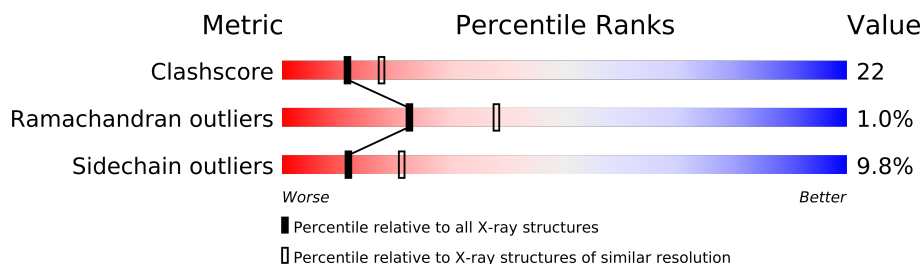
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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 2.50 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	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	N	388	
2	H	120	
3	L	104	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5124 atoms, of which 212 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	N	388	Total	C	N	O	S	8	0	0
			3067	1914	538	592	23			

- Molecule 2 is a protein called NC10 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	120	Total	C	H	N	O	S	22	0	0
			1143	585	212	153	188	5			

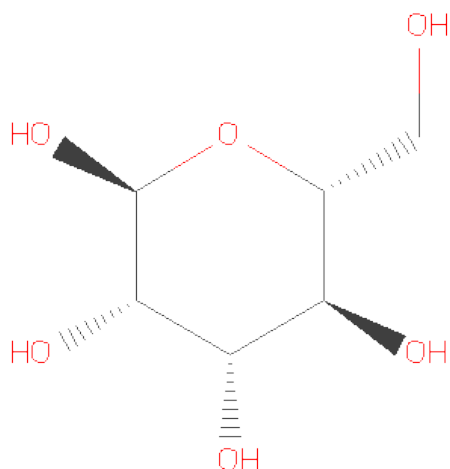
- Molecule 3 is a protein called NC10 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	104	Total	C	N	O	S	0	0	0
			802	499	129	172	2			

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

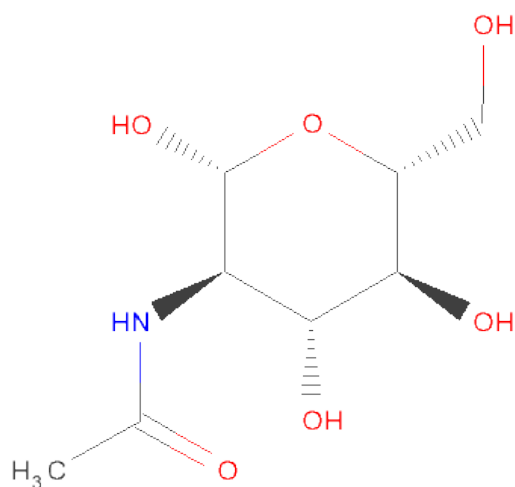
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	N	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



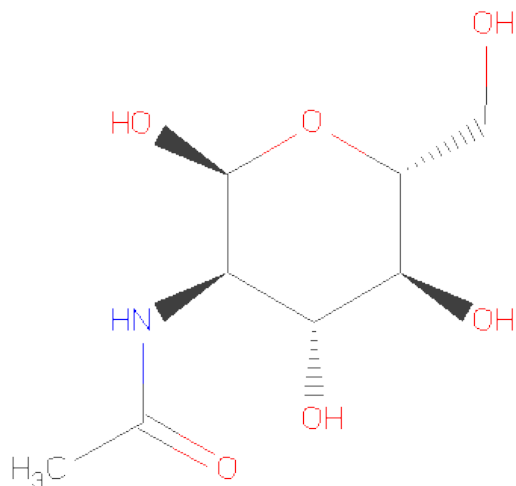
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	1	Total	Ca	0	0
			1	1		

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, α , β , γ	165.30Å 165.30Å 182.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	80.0 (7.00-2.50)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5124	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: CA, BMA, NAG, NDG, 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	0.73	0/3150	0.93	5/4290 (0.1%)
2	H	0.51	0/954	0.74	0/1290
3	L	0.58	0/818	0.70	0/1113
All	All	0.67	0/4922	0.86	5/6693 (0.1%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	189	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	N	189	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	N	299	ASN	N-CA-C	-5.95	94.94	111.00
1	N	226	GLN	N-CA-C	5.34	125.43	111.00
1	N	439	THR	N-CA-C	-5.20	96.97	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	341	TYR	Sidechain
1	N	374	TYR	Sidechain

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	N	3067	0	2892	133	0
2	H	931	212	658	42	0
3	L	802	0	748	34	0
4	N	72	0	60	2	0
5	N	11	0	9	3	0
6	N	14	0	13	0	0
7	N	14	0	13	0	0
8	N	1	0	0	0	0
All	All	4912	212	4393	208	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 22.

The worst 5 of 208 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:39:ASN:HD21	3:L:45:LYS:HD3	1.40	0.86
1:N:283:GLU:HG2	1:N:284:ARG:HG3	1.56	0.85
1:N:168:THR:HG22	1:N:170:ASN:H	1.41	0.84
1:N:141:ARG:NH2	1:N:467:PHE:HA	1.91	0.83
1:N:159:ILE:HG22	1:N:173:VAL:HA	1.60	0.81

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	N	386/388 (100%)	354 (92%)	29 (8%)	3 (1%)	27	46
2	H	118/120 (98%)	104 (88%)	13 (11%)	1 (1%)	27	46
3	L	102/104 (98%)	92 (90%)	8 (8%)	2 (2%)	11	17
All	All	606/612 (99%)	550 (91%)	50 (8%)	6 (1%)	22	38

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	148	THR
3	L	28	ASP
1	N	295	TRP
1	N	222	ILE
2	H	16	ALA

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	N	341/341 (100%)	311 (91%)	30 (9%)	14	26
2	H	98/98 (100%)	86 (88%)	12 (12%)	7	12
3	L	91/91 (100%)	81 (89%)	10 (11%)	9	16
All	All	530/530 (100%)	478 (90%)	52 (10%)	12	21

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	364	ARG
1	N	468	LEU
3	L	45	LYS
1	N	367	SER
1	N	414	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	31	ASN
3	L	38	GLN
2	H	39	GLN
1	N	345	ASN
2	H	76	ASN

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 ⓘ

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	12,14,15	1.59	3 (25%)	15,19,21	2.93	6 (40%)
4	NAG	N	470(B)	4	12,14,15	1.30	2 (16%)	15,19,21	1.67	3 (20%)
4	BMA	N	471(C)	4	10,11,12	2.46	3 (30%)	11,15,17	2.86	5 (45%)
4	MAN	N	472(D)	4	10,11,12	2.02	4 (40%)	11,15,17	1.48	2 (18%)
4	MAN	N	473(E)	4	10,11,12	1.50	1 (10%)	11,15,17	2.44	5 (45%)
4	MAN	N	474(F)	4	10,11,12	0.95	1 (10%)	11,15,17	1.30	2 (18%)

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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	471(C)	BMA	O3-C3	-5.60	1.29	1.43
4	N	471(C)	BMA	O5-C5	4.73	1.54	1.45
4	N	472(D)	MAN	C3-C2	-3.96	1.44	1.52
4	N	473(E)	MAN	C4-C3	3.47	1.61	1.52
4	N	469(A)	NAG	C4-C5	3.35	1.60	1.53

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	471(C)	BMA	O5-C5-C6	7.23	114.57	106.98
4	N	469(A)	NAG	C3-C2-N2	-6.86	101.31	111.76
4	N	469(A)	NAG	C8-C7-N2	-5.81	104.75	116.11
4	N	473(E)	MAN	O5-C5-C4	-5.20	104.05	110.65
4	N	469(A)	NAG	O7-C7-C8	4.77	131.35	122.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	MAN	N	475(G)	-	10,11,12	2.04	3 (30%)	11,15,17	3.13	7 (63%)
6	NAG	N	476(A)	1	12,14,15	1.69	3 (25%)	15,19,21	1.65	2 (13%)
7	NDG	N	477(A)	1	12,14,15	1.90	4 (33%)	15,19,21	2.15	3 (20%)

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	MAN	N	475(G)	-	-	0/2/19/22	0/1/1/1
6	NAG	N	476(A)	1	-	0/6/23/26	0/1/1/1
7	NDG	N	477(A)	1	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	475(G)	MAN	O5-C5	-4.75	1.36	1.45
7	N	477(A)	NDG	C8-C7	4.31	1.59	1.50
6	N	476(A)	NAG	C3-C2	3.27	1.59	1.52
6	N	476(A)	NAG	C4-C5	3.25	1.60	1.53
6	N	476(A)	NAG	C4-C3	3.10	1.60	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	475(G)	MAN	C3-C4-C5	5.76	120.48	110.20
7	N	477(A)	NDG	C3-C2-N2	-5.74	103.01	111.76
5	N	475(G)	MAN	O4-C4-C3	-4.69	99.83	110.35
6	N	476(A)	NAG	O5-C5-C6	-4.33	102.44	106.98
5	N	475(G)	MAN	O5-C5-C4	-4.16	105.38	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 was not executed - this section will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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