



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:53 AM GMT

PDB ID : 1NCD  
Title : REFINED CRYSTAL STRUCTURE OF THE INFLUENZA VIRUS N9  
NEURAMINIDASE-NC41 FAB COMPLEX  
Authors : Tulip, W.R.; Varghese, J.N.; Colman, P.M.  
Deposited on : 1992-01-21  
Resolution : 2.90 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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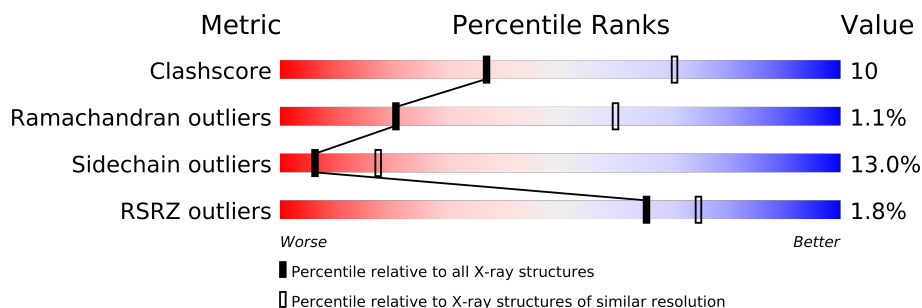
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.90 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	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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.

Mol	Chain	Length	Quality of chain
1	N	389	
2	L	214	
3	H	221	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6585 atoms, of which 0 are hydrogen 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 INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	389	Total	C	N	O	S	0	0	0
			3069	1912	539	595	23			

- Molecule 2 is a protein called IGG2A-KAPPA NC41 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1667	1043	280	336	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	20	THR	SER	CONFLICT	EMBL Y11589
L	21	ILE	VAL	CONFLICT	EMBL Y11589
L	28	ASP	ILE	CONFLICT	EMBL Y11589
L	30	SER	GLY	CONFLICT	EMBL Y11589
L	32	ALA	ASN	CONFLICT	EMBL Y11589
L	34	VAL	ALA	CONFLICT	EMBL Y11589
L	46	LEU	ALA	CONFLICT	EMBL Y11589
L	50	TRP	SER	CONFLICT	EMBL Y11589
L	53	THR	TYR	CONFLICT	EMBL Y11589
L	55	HIS	TYR	CONFLICT	EMBL Y11589
L	56	ILE	SER	CONFLICT	EMBL Y11589
L	63	ALA	THR	CONFLICT	EMBL Y11589
L	71	TYR	PHE	CONFLICT	EMBL Y11589
L	77	SER	ASN	CONFLICT	EMBL Y11589
L	80	ALA	SER	CONFLICT	EMBL Y11589
L	85	LEU	GLU	CONFLICT	EMBL Y11589
L	87	TYR	PHE	CONFLICT	EMBL Y11589
L	91	HIS	TYR	CONFLICT	EMBL Y11589
L	92	TYR	ASN	CONFLICT	EMBL Y11589
L	93	SER	ARG	CONFLICT	EMBL Y11589

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Chain	Residue	Modelled	Actual	Comment	Reference
L	94	PRO	TYR	CONFLICT	EMBL Y11589

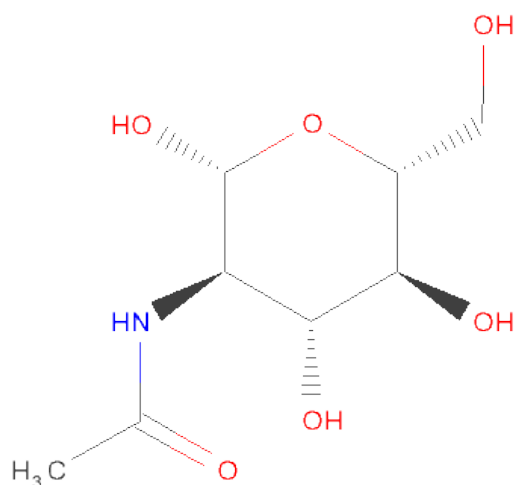
- Molecule 3 is a protein called IGG2A-KAPPA NC41 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1665	1050	273	335	7			

- 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		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

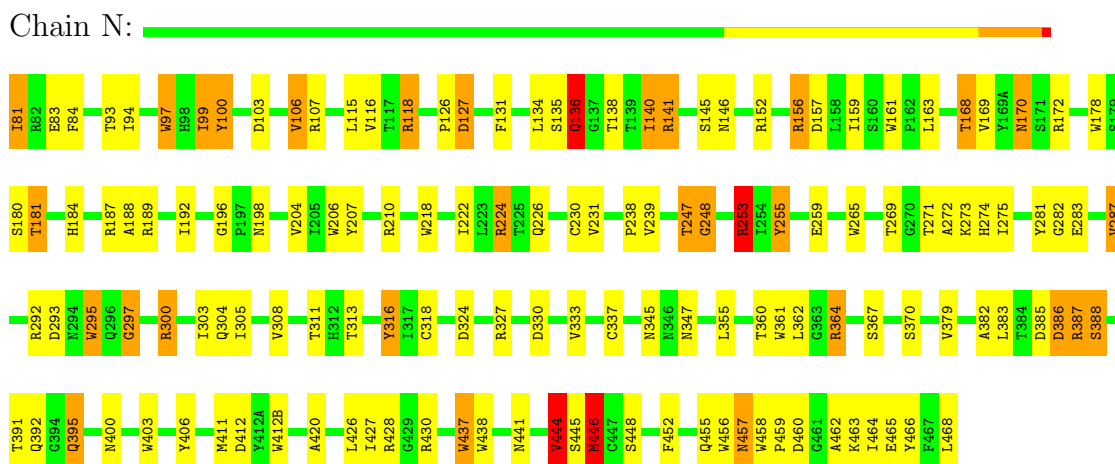
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	63	Total 63	O 63	0	0
8	L	2	Total 2	O 2	0	0
8	H	4	Total 4	O 4	0	0

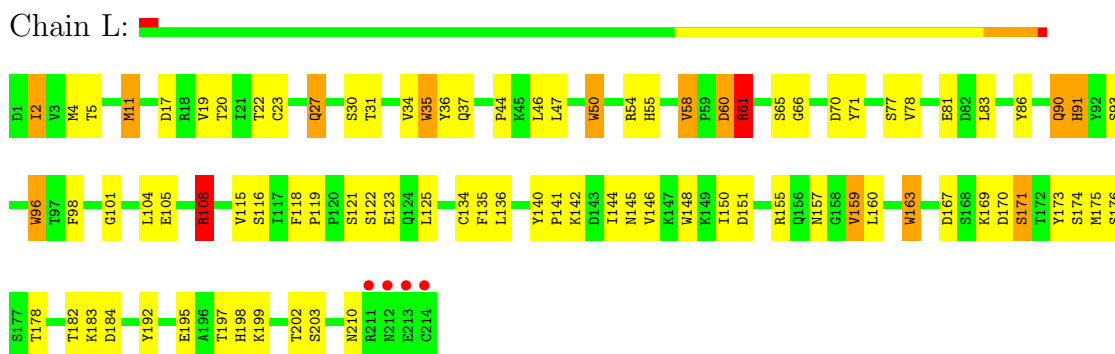
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

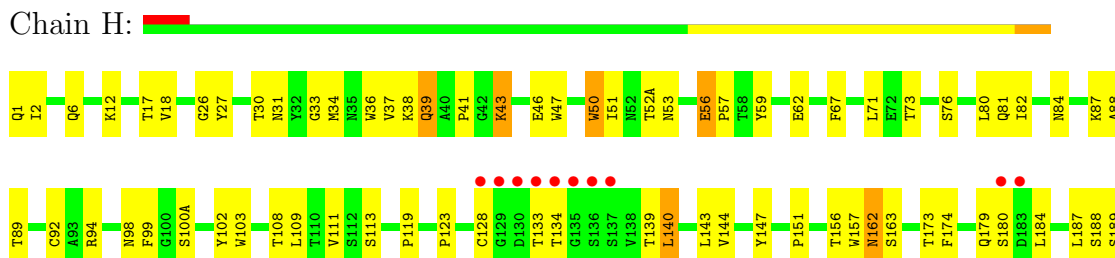
#### • Molecule 1: INFLUENZA A SUBTYPE N9 NEURAMINIDASE

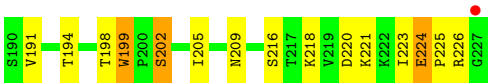


#### • Molecule 2: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)



#### • Molecule 3: IGG2A-KAPPA NC41 FAB (HEAVY CHAIN)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.00Å 167.00Å 124.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 54.1 (8.00-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.157 , (Not available) 0.234 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 22.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 31846 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	6585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: CA, 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	1.02	2/3151 (0.1%)	1.91	92/4292 (2.1%)
2	L	0.89	0/1708	1.72	32/2323 (1.4%)
3	H	0.86	0/1707	1.72	28/2326 (1.2%)
All	All	0.95	2/6566 (0.0%)	1.81	152/8941 (1.7%)

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	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	157	ASP	CB-CG	5.82	1.64	1.51
1	N	438	TRP	CD1-NE1	-5.46	1.28	1.38

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	54	ARG	NE-CZ-NH2	-14.01	113.29	120.30
1	N	224	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	N	107	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	N	300	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	N	210	ARG	NE-CZ-NH2	-9.66	115.47	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	140	TYR	Sidechain
1	N	196	GLY	Peptide
1	N	248	GLY	Peptide

## 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	3069	0	2886	62	0
2	L	1667	0	1598	38	0
3	H	1665	0	1612	34	0
4	N	72	0	61	0	0
5	N	14	0	13	0	0
6	N	28	0	25	0	0
7	N	1	0	0	0	0
8	H	4	0	0	0	0
8	L	2	0	0	0	0
8	N	63	0	0	0	0
All	All	6585	0	6195	129	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 10.

The worst 5 of 129 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:91:HIS:HB2	3:H:100(A):SER:HB2	1.65	0.77
1:N:426:LEU:HD11	1:N:444:VAL:HG22	1.67	0.75
1:N:97:TRP:H	1:N:395:GLN:HE22	1.40	0.69
2:L:108:ARG:HG3	2:L:171:SER:HB2	1.75	0.67
1:N:81:ILE:HG13	1:N:83:GLU:H	1.59	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	N	387/389 (100%)	352 (91%)	33 (8%)	2 (0%)	38	79
2	L	212/214 (99%)	197 (93%)	14 (7%)	1 (0%)	38	79
3	H	219/221 (99%)	192 (88%)	21 (10%)	6 (3%)	8	30
All	All	818/824 (99%)	741 (91%)	68 (8%)	9 (1%)	21	60

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	295	TRP
2	L	60	ASP
3	H	216	SER
3	H	226	ARG
1	N	222	ILE

### 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%)	303 (89%)	38 (11%)	9	26
2	L	190/190 (100%)	160 (84%)	30 (16%)	4	11
3	H	187/187 (100%)	162 (87%)	25 (13%)	6	15
All	All	718/718 (100%)	625 (87%)	93 (13%)	6	17

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	27	GLN

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Mol	Chain	Res	Type
2	L	105	GLU
3	H	184	LEU
2	L	58	VAL
2	L	70	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	441	ASN
1	N	457	ASN
3	H	53	ASN
1	N	395	GLN
3	H	82(B)	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 ⓘ

8 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	0.85	0	15,19,21	1.37	2 (13%)
4	NAG	N	470(B)	4	12,14,15	0.72	0	15,19,21	1.53	2 (13%)
4	BMA	N	471(C)	4	10,11,12	1.20	1 (10%)	11,15,17	2.36	4 (36%)
4	MAN	N	472(D)	4	10,11,12	1.05	0	11,15,17	1.44	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	N	473(E)	4	10,11,12	1.18	1 (10%)	11,15,17	1.41	1 (9%)
4	MAN	N	474(F)	4	10,11,12	1.24	2 (20%)	11,15,17	0.95	0
6	NAG	N	476(A)	1,6	12,14,15	0.84	0	15,19,21	1.45	3 (20%)
6	NAG	N	477(B)	6	12,14,15	0.84	0	15,19,21	2.29	4 (26%)

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
6	NAG	N	476(A)	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	477(B)	6	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	473(E)	MAN	C3-C2	2.77	1.59	1.52
4	N	474(F)	MAN	O3-C3	-2.12	1.37	1.43
4	N	471(C)	BMA	O5-C5	-2.06	1.41	1.45
4	N	474(F)	MAN	C3-C2	-2.01	1.48	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	477(B)	NAG	C3-C2-N2	-5.88	102.81	111.76
4	N	471(C)	BMA	O5-C5-C4	-5.03	104.27	110.65
6	N	477(B)	NAG	C2-N2-C7	3.60	129.13	123.09
4	N	471(C)	BMA	O5-C5-C6	3.46	110.61	106.98
4	N	470(B)	NAG	C3-C2-N2	-3.27	106.79	111.76

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	477(B)	NAG	C1-C2-N2-C7

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	N	475(A)	1	12,14,15	0.83	0	15,19,21	1.41	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	N	475(A)	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	475(A)	NAG	C8-C7-N2	3.21	122.37	116.11

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	N	389/389 (100%)	-1.01	0 100 100	2, 8, 24, 47	0
2	L	214/214 (100%)	-0.39	4 (1%) 64 72	4, 25, 42, 47	0
3	H	221/221 (100%)	-0.34	11 (4%) 28 33	4, 26, 40, 45	0
All	All	824/824 (100%)	-0.67	15 (1%) 65 74	2, 17, 38, 47	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	128	CYS	8.4
2	L	214	CYS	7.8
3	H	134	THR	6.5
3	H	135	GLY	6.3
3	H	129	GLY	5.7

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

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

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	N	477(B)	14/15	0.23	-	54,57,59,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	N	469(A)	14/15	0.11	-	5,11,23,24	0
4	MAN	N	473(E)	11/12	0.15	-	14,17,19,19	0
4	MAN	N	472(D)	11/12	0.12	-	9,11,14,19	0
4	NAG	N	470(B)	14/15	0.11	-	12,14,16,20	0
6	NAG	N	476(A)	14/15	0.23	-	41,46,53,57	0
4	BMA	N	471(C)	11/12	0.12	-	8,11,13,13	0
4	MAN	N	474(F)	11/12	0.12	-	11,13,15,16	0

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CA	N	0	1/1	0.08	-	20,20,20,20	0
5	NAG	N	475(A)	14/15	0.20	-	37,40,44,46	0

## 6.5 Other polymers

There are no such residues in this entry.