

# Full wwPDB Geometry-Only Validation Report (i)

### Feb 18, 2024 – 11:57 PM EST

PDB ID	:	4HYA
Title	:	HYALURONIC ACID, THE ROLE OF DIVALENT CATIONS IN CONFOR-
		MATION AND PACKING
Authors	:	Arnott, S.
Deposited on		
Resolution	:	3.00 Å(reported)

This is a Full wwPDB Geometry-Only Validation Report for a publicly released PDB entry.

We welcome your comments at 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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)	:	2.36

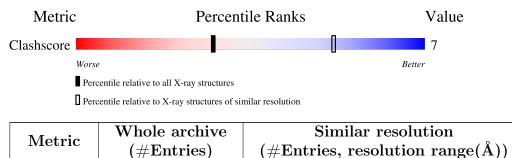
## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $FIBER\ DIFFRACTION$ 

The reported resolution of this entry is 3.00 Å.

141614

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.



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 of the lower bar indicate
the fraction of residues that contain outliers for $>=3, 2, 1$ 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 $\leq =5\%$

2416(3.00-3.00)

Note EDS was not executed.

Clashscore

Mol	Chain	Length		Quality of chain	
1	А	6	33%	67%	-

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	GCU	А	1	Х	-	-	-
1	GCU	А	3	Х	-	-	-
1	GCU	А	5	Х	-	-	-



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 138 atoms, of which 48 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 an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alp ha-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D -glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-gluc opyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	6	Total 126	C 42	Н 48	N 3	O 33	0	0	0

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	3	Total Ca 3 3	0	0

• Molecule 3 is water.

I	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	А	9	Total O 9 9	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: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-3)-2-aceta mido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranuronic acid

Chain A:	33%	67%
GCU1 NAG2 GCU3 NAG4 CCU5 NAG6		



## 4 Model quality (i)

## 4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GCU, CA

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 4.2 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	А	78	48	55	1	1
2	А	3	0	0	0	0
3	А	9	0	0	0	0
All	All	90	48	55	1	1

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 7.

All (1) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Atom-2 Interatomic distance (Å)	
1:A:3:GCU:O3	1:A:4:NAG:C1	2.66	0.43

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GCU:O1	1:A:6:NAG:C3[1_554]	1.43	0.77

### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

There are no protein molecules in this entry.

#### 4.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

## 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

## 4.5 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	Turne	Chain	Res	Link	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
INIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	GCU	А	1	$^{2,1}$	13,13,13	0.56	0	18,19,19	0.81	1 (5%)
1	NAG	А	2	1	14,14,15	0.51	0	17,19,21	0.91	1 (5%)
1	GCU	А	3	2,1	12,12,13	0.61	0	14,17,19	0.91	1 (7%)
1	NAG	А	4	1	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
1	GCU	А	5	2,1	12,12,13	0.88	1 (8%)	14,17,19	0.97	1 (7%)



Mol	Type	Chain	Res	Link	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
Moi Type C	Unam	I nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
1	NAG	А	6	1	13,13,15	0.58	0	$16,\!17,\!21$	1.13	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
1	GCU	А	1	2,1	1/1/6/6	2/4/24/24	0/1/1/1
1	NAG	А	2	1	-	2/6/23/26	0/1/1/1
1	GCU	А	3	2,1	1/1/6/6	4/4/21/24	0/1/1/1
1	NAG	А	4	1	-	2/6/23/26	0/1/1/1
1	GCU	А	5	2,1	1/1/6/6	2/4/21/24	0/1/1/1
1	NAG	А	6	1	-	2/6/19/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	5	GCU	C5-C6	-2.10	1.48	1.53

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	6	NAG	C2-N2-C7	-2.97	118.88	122.78
1	А	4	NAG	C2-N2-C7	-2.85	118.84	122.90
1	А	2	NAG	C2-N2-C7	-2.76	118.98	122.90
1	А	5	GCU	O6B-C6-O6A	2.63	130.06	124.09
1	А	1	GCU	O6B-C6-O6A	2.60	130.00	124.09
1	А	3	GCU	O6B-C6-O6A	2.56	129.90	124.09

All (6) bond angle outliers are listed below:

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	А	1	GCU	C1
1	А	3	GCU	C1
1	А	5	GCU	C1

All (14) torsion outliers are listed below:



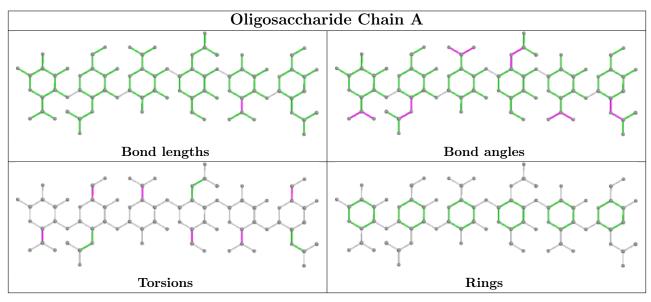
Mol	Chain	Res	Type	Atoms
1	А	1	GCU	C4-C5-C6-O6A
1	А	1	GCU	C4-C5-C6-O6B
1	А	6	NAG	C4-C5-C6-O6
1	А	4	NAG	O5-C5-C6-O6
1	А	6	NAG	O5-C5-C6-O6
1	А	2	NAG	O5-C5-C6-O6
1	А	2	NAG	C4-C5-C6-O6
1	А	4	NAG	C4-C5-C6-O6
1	А	3	GCU	C4-C5-C6-O6A
1	А	3	GCU	C4-C5-C6-O6B
1	А	3	GCU	O5-C5-C6-O6A
1	А	3	GCU	O5-C5-C6-O6B
1	А	5	GCU	O5-C5-C6-O6A
1	А	5	GCU	O5-C5-C6-O6B

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	1	GCU	0	1
1	А	6	NAG	0	1
1	А	4	NAG	1	0
1	А	3	GCU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 4.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers. There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

