WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB Geometry-Only Validation Summary Report ⓘ

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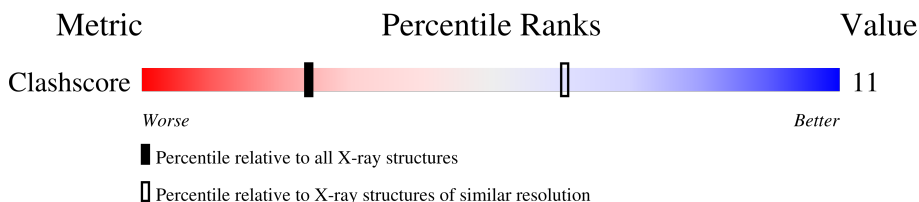|		
PDB ID	:	3HYA
Title	:	HYALURONIC ACID, MOLECULAR CONFORMATIONS AND INTERACTIONS IN TWO SODIUM SALTS
Authors	:	Arnott, S.
Deposited on	:	1977-11-20
Resolution	:	3.00 Å(reported)

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
FIBER 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	Percentile Ranks	Value
Clashscore		11

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	8	100%

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	A	1	-	-	X	-
1	NAG	A	2	-	-	X	-
1	BDP	A	3	-	-	X	-
1	NAG	A	4	-	-	X	-
1	BDP	A	5	-	-	X	-
1	NAG	A	6	-	-	X	-
1	BDP	A	7	-	-	X	-
1	NAG	A	8	-	-	X	-
2	NA	A	10	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	A	12	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 180 atoms, of which 64 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)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranuronic acid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	8	Total	C	H	N	O	0	0	0
			168	56	64	4	44			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Na	0	0
			4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		

3 Residue-property plots ⓘ

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)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranuronic acid

Chain A: 100%

GCU1 NAG2 BDP3 NAG4 BDP5 NAG6 BDP7 NAG8

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

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 ⓘ

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	A	104	64	73	2	218
2	A	4	0	0	0	6
3	A	8	0	0	0	36
All	All	116	64	73	2	218

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 11.

All (2) 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)
1:A:3:BDP:O6A	1:A:4:NAG:C1	2.59	0.51
1:A:7:BDP:O6A	1:A:8:NAG:C1	2.59	0.50

The worst 5 of 218 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:O2	1:A:4:NAG:C2[3_545]	0.46	1.74
1:A:5:BDP:O2	1:A:8:NAG:C2[3_556]	0.46	1.74
1:A:1:GCU:C1	1:A:4:NAG:C7[3_545]	0.50	1.70
1:A:5:BDP:C1	1:A:8:NAG:C7[3_556]	0.50	1.70
1:A:4:NAG:C6	1:A:8:NAG:C6[3_546]	0.53	1.67

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

4.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

8 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
1	GCU	A	1	1,2	12,12,13	0.61	0	14,17,19	0.91	1 (7%)
1	NAG	A	2	1	14,14,15	0.50	0	17,19,21	0.91	1 (5%)
1	BDP	A	3	1,2	12,12,13	0.60	0	14,17,19	0.92	1 (7%)
1	NAG	A	4	1	14,14,15	0.51	0	17,19,21	0.93	1 (5%)
1	BDP	A	5	1,2	12,12,13	0.61	0	14,17,19	0.91	1 (7%)
1	NAG	A	6	1	14,14,15	0.50	0	17,19,21	0.91	1 (5%)
1	BDP	A	7	1,2	12,12,13	0.60	0	14,17,19	0.92	1 (7%)
1	NAG	A	8	1	14,14,15	0.51	0	17,19,21	0.93	1 (5%)

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	A	1	1,2	-	0/4/21/24	0/1/1/1
1	NAG	A	2	1	-	1/6/23/26	0/1/1/1
1	BDP	A	3	1,2	-	2/4/21/24	0/1/1/1
1	NAG	A	4	1	-	1/6/23/26	0/1/1/1
1	BDP	A	5	1,2	-	0/4/21/24	0/1/1/1
1	NAG	A	6	1	-	1/6/23/26	0/1/1/1
1	BDP	A	7	1,2	-	2/4/21/24	0/1/1/1
1	NAG	A	8	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	NAG	C2-N2-C7	-2.82	118.89	122.90
1	A	8	NAG	C2-N2-C7	-2.82	118.89	122.90
1	A	2	NAG	C2-N2-C7	-2.77	118.96	122.90
1	A	6	NAG	C2-N2-C7	-2.77	118.96	122.90
1	A	3	BDP	O6B-C6-O6A	2.60	129.99	124.09

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
1	A	4	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
1	A	8	NAG	C4-C5-C6-O6
1	A	2	NAG	C4-C5-C6-O6
1	A	6	NAG	C4-C5-C6-O6
1	A	3	BDP	O5-C5-C6-O6B

There are no ring outliers.

8 monomers are involved in 220 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4	NAG	1	73
1	A	6	NAG	0	40
1	A	7	BDP	1	34
1	A	5	BDP	0	48
1	A	8	NAG	1	74
1	A	1	GCU	0	49
1	A	3	BDP	1	34
1	A	2	NAG	0	40

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

Oligosaccharide Chain A

Bond lengths   Bond angles

Torsions   Rings
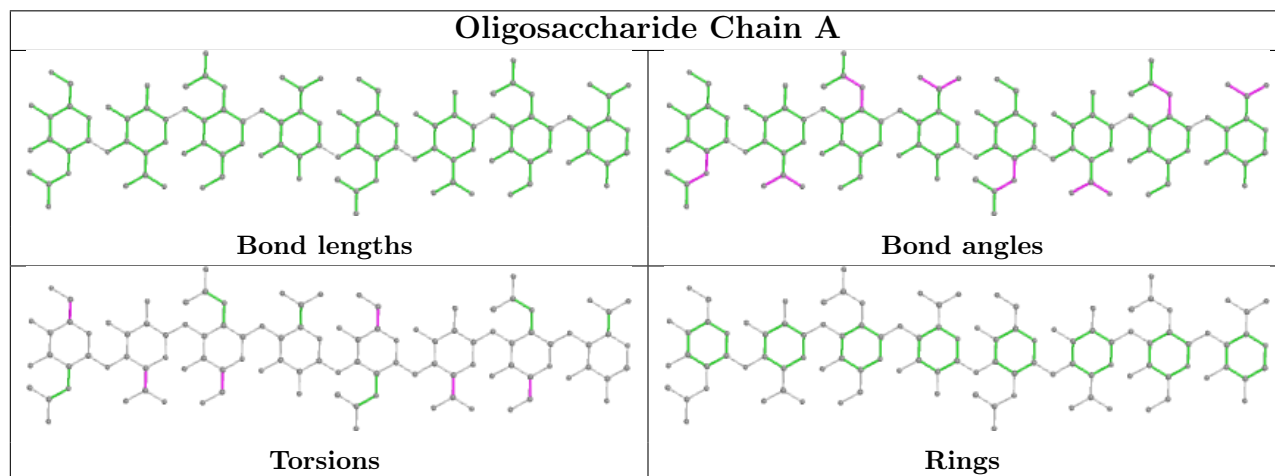
4.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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 ⓘ

There are no such residues in this entry.

4.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.