



Full wwPDB Geometry-Only Validation Report ⓘ

Aug 8, 2020 – 07:09 AM BST

PDB ID : 1KES
Title : CONFORMATION OF KERATAN SULPHATE
Authors : Arnott, S.
Deposited on : 1978-05-23
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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) : 2.13.1

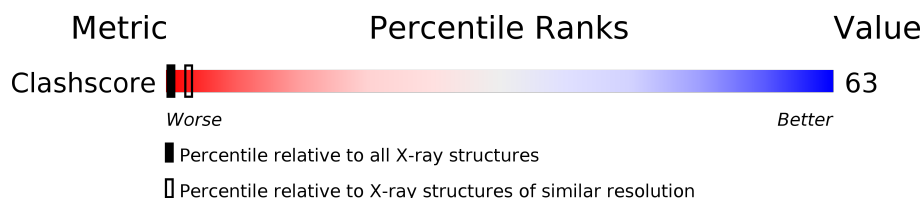
1 Overall quality at a glance

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	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 on 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 $\leq 5\%$

Note EDS was not executed.

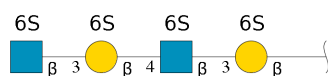
Mol	Chain	Length	Quality of chain
1	A	4	 100%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 66 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 an oligosaccharide called 2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranoside-(1-3)-6-O-sulfo-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose-(1-3)-6-O-sulfo-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	4	Total	C	N	O	S	0	0	0
			66	28	2	32	4			

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-6-O-sulfo-beta-D-glucopyranose-(1-3)-6-O-sulfo-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose-(1-3)-6-O-sulfo-beta-D-galactopyranose

Chain A:  100%

66S1
66S2
66S3
66S4

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: G6S, NGS

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	A	66	0	29	6	0
All	All	66	0	29	6	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 63.

All (6) 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:1:G6S:O2	1:A:2:NGS:C7	2.61	0.48
1:A:1:G6S:O2	1:A:2:NGS:C8	2.62	0.48
1:A:3:G6S:O2	1:A:4:NGS:C7	2.61	0.48
1:A:1:G6S:O2	1:A:2:NGS:N2	2.47	0.48
1:A:3:G6S:O2	1:A:4:NGS:C8	2.62	0.47
1:A:3:G6S:O2	1:A:4:NGS:N2	2.47	0.47

There are no symmetry-related clashes.

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](#)

4 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	G6S	A	1	1	16,16,16	0.46	0	22,24,24	0.66	1 (4%)
1	NGS	A	2	1	18,18,19	0.60	0	22,26,28	0.99	2 (9%)
1	G6S	A	3	1	15,15,16	0.48	0	20,22,24	0.68	1 (5%)
1	NGS	A	4	1	17,17,19	0.64	0	19,24,28	1.08	2 (10%)

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	G6S	A	1	1	-	0/6/26/26	0/1/1/1
1	NGS	A	2	1	-	0/10/27/30	0/1/1/1
1	G6S	A	3	1	-	0/6/23/26	0/1/1/1
1	NGS	A	4	1	-	0/10/23/30	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	NGS	C2-N2-C7	-2.81	118.90	122.90
1	A	2	NGS	C2-N2-C7	-2.81	118.90	122.90
1	A	4	NGS	O6-C6-C5	2.30	111.81	107.70
1	A	2	NGS	O6-C6-C5	2.24	111.81	107.62
1	A	1	G6S	O6-C6-C5	2.24	111.80	107.62
1	A	3	G6S	O6-C6-C5	2.24	111.80	107.62

There are no chirality outliers.

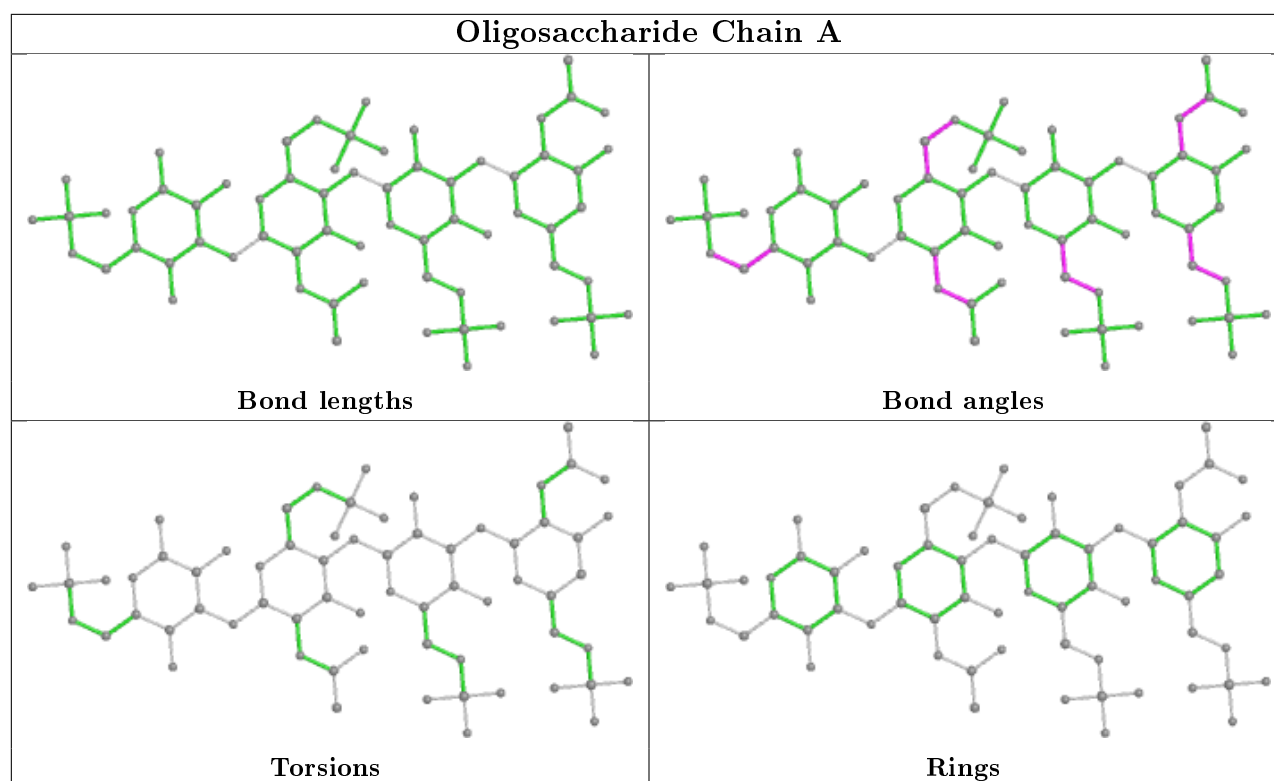
There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4	NGS	3	0
1	A	1	G6S	3	0
1	A	2	NGS	3	0
1	A	3	G6S	3	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](#)

There are no ligands in this entry.

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.