wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 02:10 AM EDT

PDB ID	:	6VU6
Title	:	Sialic acid binding region of Streptococcus Sanguinis SK1 adhesin bound to 3'sLn
Authors	:	Stubbs, H.E.; Iverson, T.M.
Deposited on	:	2020-02-14
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6792 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 a protein called Adhesin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	409	Total 3136	C 1947	N 545	O 644	0	0	0
1	E	409	Total 3147	C 1953	N 549	O 645	0	1	0

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total 46	C 25	N 2	O 19	0	0	0
2	C	3	Total 46	C 25	N 2	O 19	0	0	0
2	D	3	Total 46	C 25	N 2	O 19	0	0	0
2	F	3	Total 46	C 25	N 2	O 19	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	Ca 4	0	0
3	E	4	Total 4	Ca 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	174	Total 174	O 174	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	143	Total 143	O 143	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	82.21Å 269.86Å 47.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.10 – 2.10	Depositor
% Data completeness (in resolution range)	87.4 (35.10-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.225 , 0.248	Depositor
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.450	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6792	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

12 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	$\#\|Z\|>2$
2	NAG	B	1	2	15,15,15	0.58	0	21,21,21	0.77	1 (4%)
2	GAL	B	2	2	11,11,12	1.40	1 (9%)	15,15,17	1.65	2 (13%)
2	SIA	B	3	2	20,20,21	2.98	2 (10%)	24,28,31	1.68	3 (12%)
2	NAG	C	1	2	15,15,15	0.20	0	21,21,21	0.39	0
2	GAL	C	2	2	11,11,12	1.02	1 (9%)	15,15,17	0.98	2 (13%)
2	SIA	C	3	2	20,20,21	2.52	2 (10%)	24,28,31	1.81	5 (20%)
2	NAG	D	1	2	15,15,15	0.32	0	21,21,21	0.51	0
2	GAL	D	2	2	11,11,12	0.72	0	15,15,17	0.92	1 (6%)
2	SIA	D	3	2	20,20,21	2.43	4 (20%)	24,28,31	1.78	8 (33%)
2	NAG	F	1	2	15,15,15	0.30	0	21,21,21	0.56	0
2	GAL	F	2	2	11,11,12	0.90	0	15,15,17	1.48	3 (20%)
2	SIA	F	3	2	20,20,21	2.59	3 (15%)	24,28,31	1.56	3 (12%)

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
2	NAG	B	1	2	-	4/6/26/26	0/1/1/1
2	GAL	B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	B	3	2	-	2/18/34/38	0/1/1/1
2	NAG	C	1	2	-	2/6/26/26	0/1/1/1
2	GAL	C	2	2	-	2/2/19/22	0/1/1/1
2	SIA	C	3	2	-	3/18/34/38	0/1/1/1
2	NAG	D	1	2	-	2/6/26/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	8/18/34/38	0/1/1/1
2	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	1/2/19/22	0/1/1/1
2	SIA	F	3	2	-	3/18/34/38	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	SIA	C2-C1	12.45	1.63	1.52
2	F	3	SIA	C2-C1	10.12	1.61	1.52
2	C	3	SIA	C2-C1	9.94	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	SIA	C2-C1	8.93	1.60	1.52
2	B	2	GAL	O5-C1	-3.68	1.37	1.43

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	SIA	O6-C2-C3	-5.05	103.51	110.46
2	C	3	SIA	O6-C2-C3	-4.72	103.96	110.46
2	F	3	SIA	O6-C2-C3	-4.35	104.47	110.46
2	F	2	GAL	C1-O5-C5	3.77	117.30	112.19
2	B	2	GAL	O5-C5-C6	-3.75	101.33	107.20

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

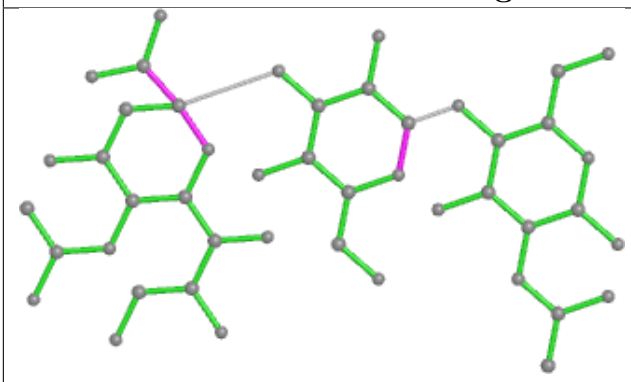
Mol	Chain	Res	Type	Atoms
2	B	3	SIA	O8-C8-C9-O9
2	D	3	SIA	C6-C7-C8-C9
2	D	3	SIA	O7-C7-C8-C9
2	D	3	SIA	O7-C7-C8-O8
2	D	2	GAL	O5-C5-C6-O6

There are no ring outliers.

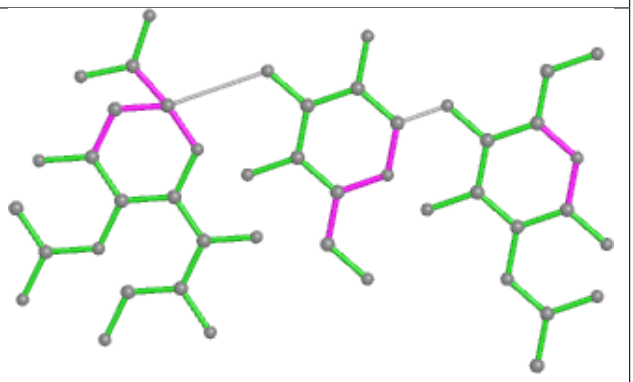
No monomer is involved in short contacts.

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

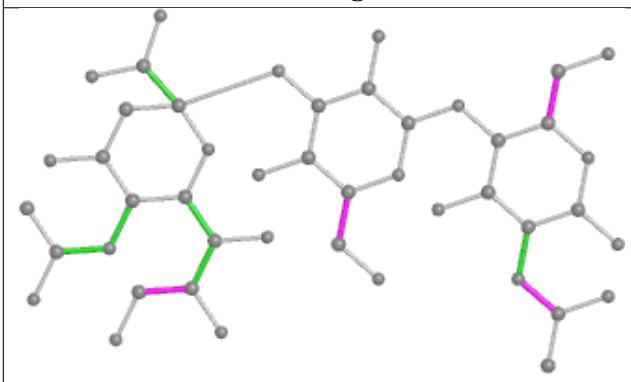
Oligosaccharide Chain B



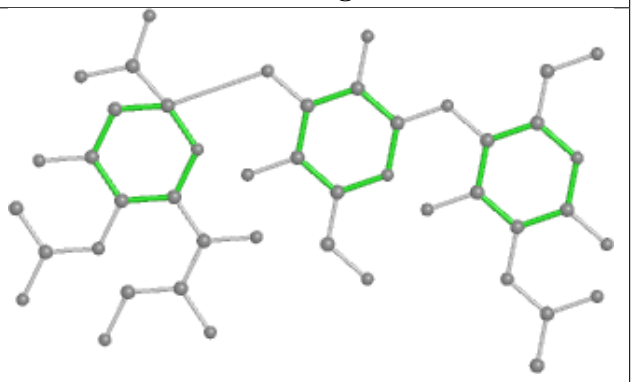
Bond lengths



Bond angles

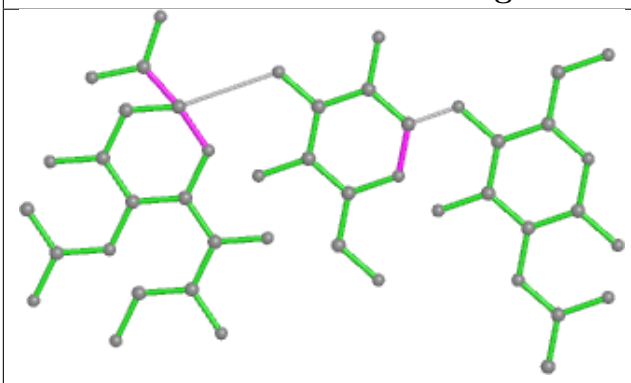


Torsions

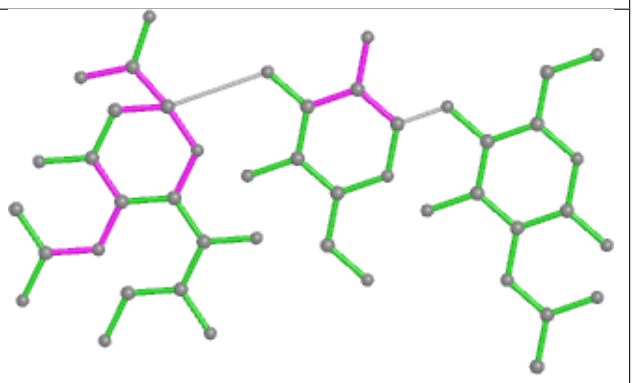


Rings

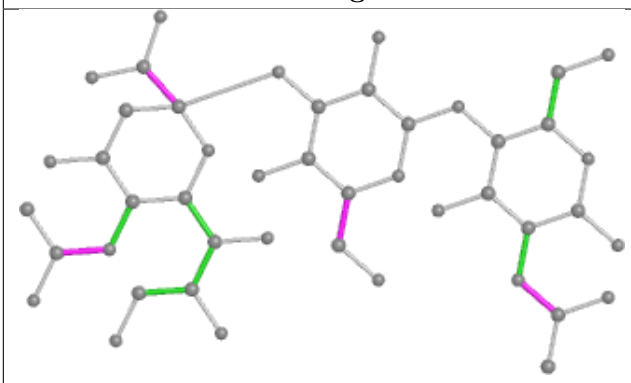
Oligosaccharide Chain C



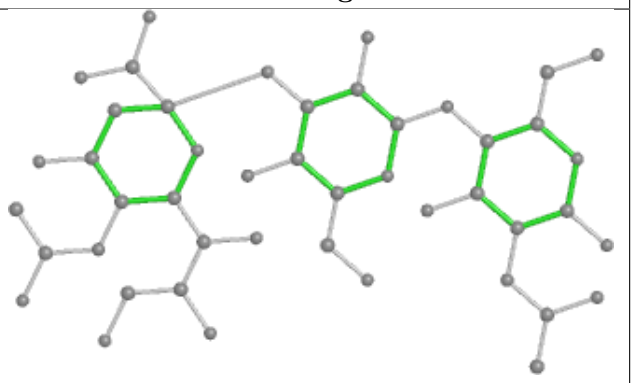
Bond lengths



Bond angles

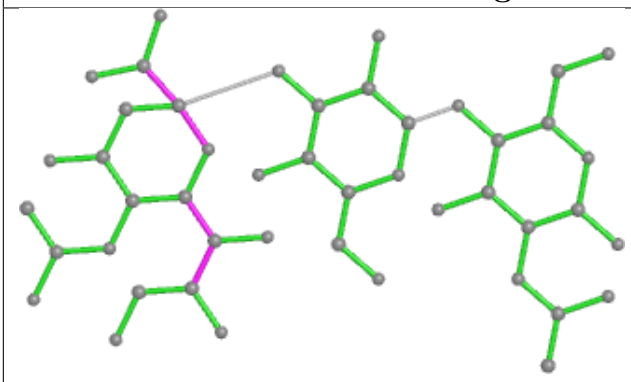


Torsions

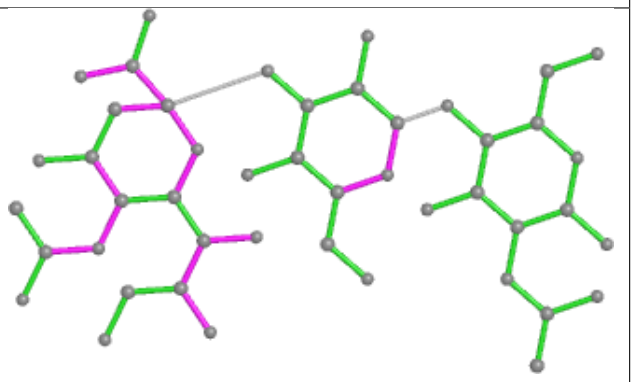


Rings

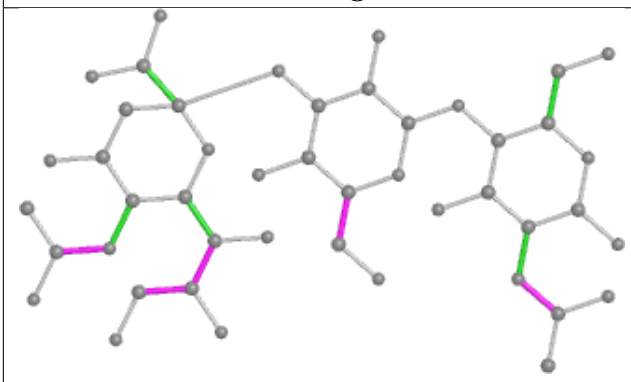
Oligosaccharide Chain D



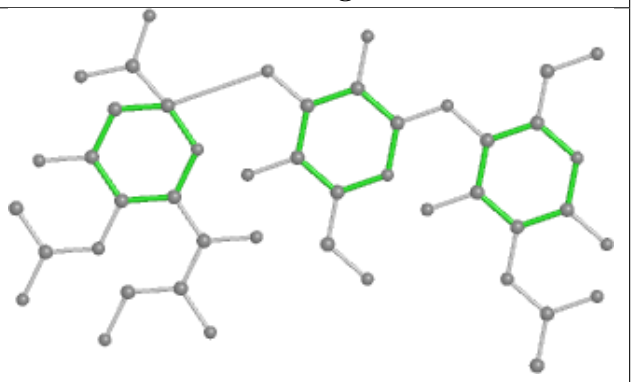
Bond lengths



Bond angles

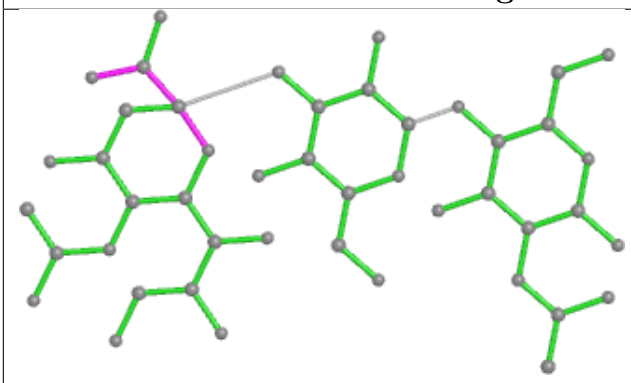


Torsions

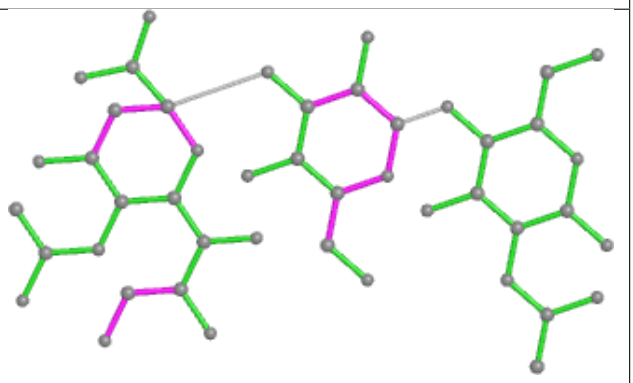


Rings

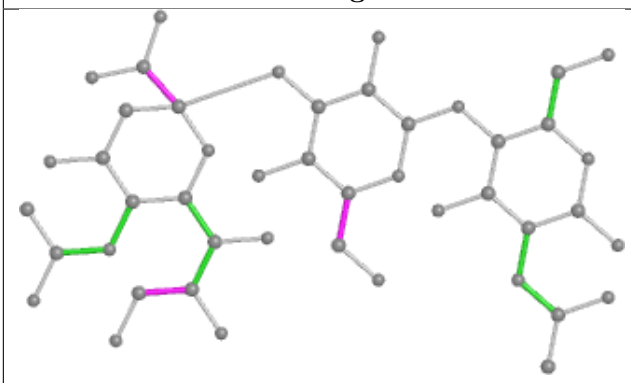
Oligosaccharide Chain F



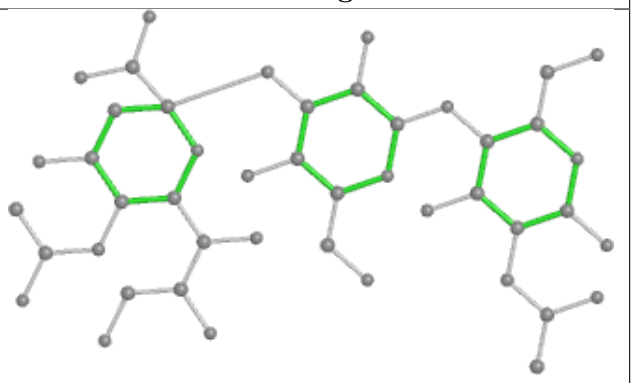
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.