Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:54 AM EDT

PDB ID	:	6MNA
Title	:	Crystal structure of LpqN involved in cell envelope biogenesis of Mycobacterium tuberculosis
Authors	:	Rajavel, M.; Su, C.C.; Yu, E.W.
Deposited on	:	2018-10-01
Resolution	:	1.75 Å(reported)

The following versions of software and data (see references ⓘ) 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 1.75 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 ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2736 atoms, of which 1304 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 Probable conserved lipoprotein LpqN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	173	Total 2559	C 818	H 1262	N 215	O 262	S 2	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	HIS	-	expression tag	UNP O53780
A	230	HIS	-	expression tag	UNP O53780
A	231	HIS	-	expression tag	UNP O53780
A	232	HIS	-	expression tag	UNP O53780
A	233	HIS	-	expression tag	UNP O53780
A	234	HIS	-	expression tag	UNP O53780

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-6-O-decanoyl-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total 76	C 22	H 42	O 12	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total 101	O 101	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	I 4	Depositor
Cell constants a, b, c, α, β, γ	79.55Å 79.55Å 59.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.25 – 1.75	Depositor
% Data completeness (in resolution range)	99.2 (56.25-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.14rc1_3177: ???)	Depositor
R, R_{free}	0.184 , 0.217	Depositor
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.379	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.038 for -k,-h,-l	Xtriage
Total number of atoms	2736	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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 ⓘ

2 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	U2D	B	1	2	22,22,23	2.11	6 (27%)	27,27,29	2.19	8 (29%)
2	GLC	B	2	2	12,12,12	0.69	0	17,17,17	0.61	0

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	U2D	B	1	2	-	3/14/31/34	0/1/1/1
2	GLC	B	2	2	-	1/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U2D	O11-CAX	7.00	1.43	1.22
2	B	1	U2D	O6-CAX	3.74	1.44	1.33
2	B	1	U2D	C1-C2	2.94	1.58	1.52
2	B	1	U2D	C2-C3	2.81	1.56	1.52
2	B	1	U2D	C4-C5	2.41	1.58	1.53
2	B	1	U2D	O5-C5	2.04	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	U2D	C3-C4-C5	-4.86	101.57	110.24
2	B	1	U2D	O6-CAX-O11	-4.21	112.97	123.59
2	B	1	U2D	O11-CAX-CAY	-3.62	109.60	123.73
2	B	1	U2D	C2-C3-C4	-3.44	104.94	110.89
2	B	1	U2D	C1-O5-C5	-3.04	108.08	112.19
2	B	1	U2D	CBC-CBB-CBA	-3.03	99.05	114.42
2	B	1	U2D	O6-C6-C5	-2.28	103.59	108.43
2	B	1	U2D	O2-C2-C1	2.13	113.52	109.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	U2D	CAY-CAX-O6-C6
2	B	1	U2D	CAY-CAZ-CBA-CBB
2	B	2	GLC	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1	U2D	O11-CAX-O6-C6

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
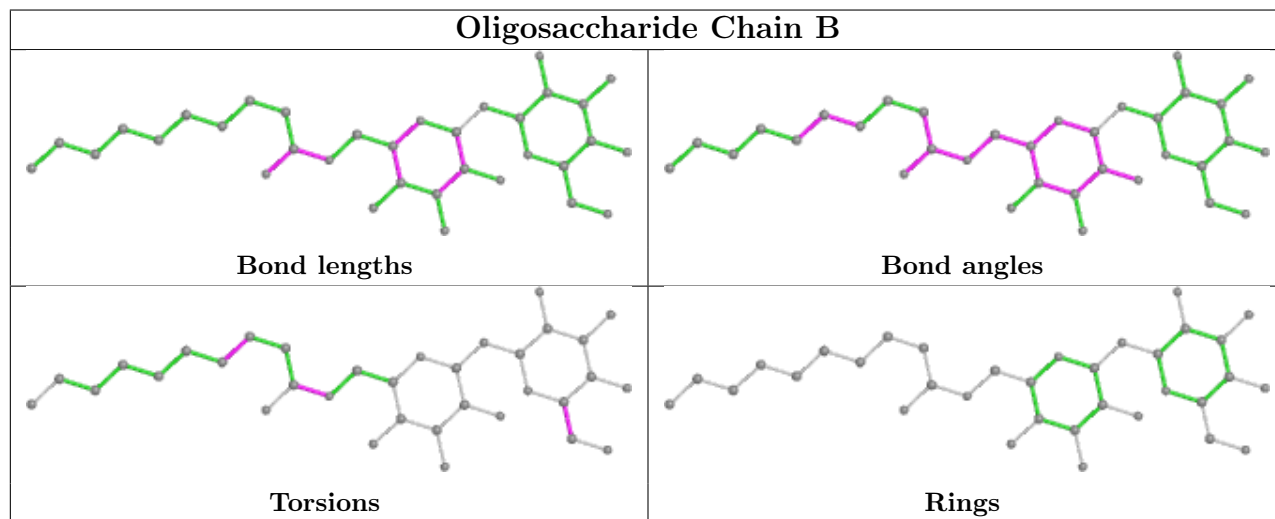
4.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.