



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:28 PM UTC

PDB ID : 4LBJ / pdb_00004bj
Title : Crystal structure of Human galectin-3 CRD K176L mutant in complex with LNT
Authors : Bum-Erdene, K.; Blanchard, H.
Deposited on : 2013-06-20
Resolution : 1.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : **FAILED**
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

PERCENTILES INFOmissingINFO

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

GLOBAL-STATISTICS INFOmissingINFO

1 Model quality [i](#)

1.1 Standard geometry [i](#)

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

1.2 Too-close contacts [i](#)

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

1.3 Torsion angles [i](#)

1.3.1 Protein backbone [i](#)

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

1.3.2 Protein sidechains [i](#)

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

1.3.3 RNA [i](#)

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

1.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

SUGAR-GEOMETRY INFOmissingINFO

1.5 Ligand geometry [i](#)

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

1.6 Other polymers [i](#)

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

1.7 Polymer linkage issues

There are no chain breaks in this entry.

2 Fit of model and data [i](#)

2.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	32/138 (23%)	-0.22	1 (3%) 51 51	5, 10, 22, 43	3 (9%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	113	MET	3.5

2.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

SUGAR-RSR INFOmissingINFO

LIGAND-RSR INFOmissingINFO

OTHERPOLY-RSR INFOmissingINFO