



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:00 PM UTC

PDB ID : 4LBJ / pdb\_00004lbj  
Title : Crystal structure of Human galectin-3 CRD K176L mutant in complex with LNT  
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Deposited on : 2013-06-20  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

### 2.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> ) | 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

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

SUGAR-RSR INFOmissingINFO

LIGAND-RSR INFOmissingINFO

OTHERPOLY-RSR INFOmissingINFO