



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2025 – 06:33 PM JST

PDB ID : 9WFH / pdb\_00009wfh  
Title : Carbohydrate-binding module 32 of LnbB from Bifidobacterium bifidum, lig-  
and free form, multiple small-wedge data set  
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Deposited on : 2025-08-21  
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

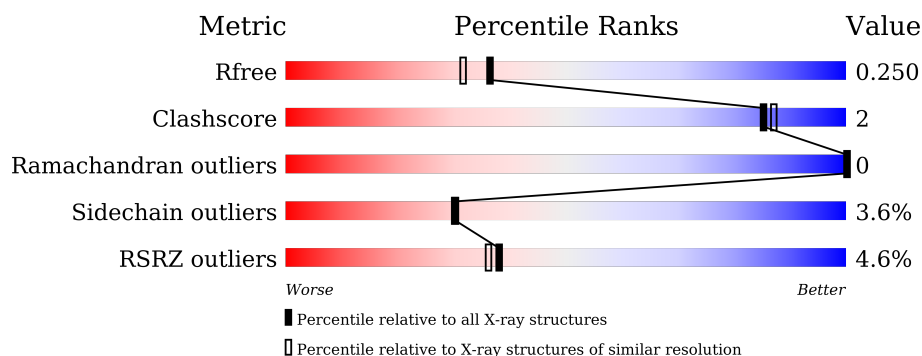
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	183	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>8% .. 12%</div> </div> </div>
1	B	183	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>7% • 11%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2568 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 Lacto-N-biosidase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	0	0	0
			1212	768	202	242			
1	B	162	Total	C	N	O	0	0	0
			1218	771	204	243			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	756	MET	-	initiating methionine	UNP B3TLD6
A	757	GLY	-	expression tag	UNP B3TLD6
A	758	SER	-	expression tag	UNP B3TLD6
A	759	SER	-	expression tag	UNP B3TLD6
A	760	HIS	-	expression tag	UNP B3TLD6
A	761	HIS	-	expression tag	UNP B3TLD6
A	762	HIS	-	expression tag	UNP B3TLD6
A	763	HIS	-	expression tag	UNP B3TLD6
A	764	HIS	-	expression tag	UNP B3TLD6
A	765	HIS	-	expression tag	UNP B3TLD6
A	766	SER	-	expression tag	UNP B3TLD6
A	767	SER	-	expression tag	UNP B3TLD6
A	768	GLY	-	expression tag	UNP B3TLD6
A	769	LEU	-	expression tag	UNP B3TLD6
A	770	VAL	-	expression tag	UNP B3TLD6
A	771	PRO	-	expression tag	UNP B3TLD6
A	772	ARG	-	expression tag	UNP B3TLD6
A	773	GLY	-	expression tag	UNP B3TLD6
A	774	SER	-	expression tag	UNP B3TLD6
B	756	MET	-	initiating methionine	UNP B3TLD6
B	757	GLY	-	expression tag	UNP B3TLD6
B	758	SER	-	expression tag	UNP B3TLD6
B	759	SER	-	expression tag	UNP B3TLD6
B	760	HIS	-	expression tag	UNP B3TLD6
B	761	HIS	-	expression tag	UNP B3TLD6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	762	HIS	-	expression tag	UNP B3TLD6
B	763	HIS	-	expression tag	UNP B3TLD6
B	764	HIS	-	expression tag	UNP B3TLD6
B	765	HIS	-	expression tag	UNP B3TLD6
B	766	SER	-	expression tag	UNP B3TLD6
B	767	SER	-	expression tag	UNP B3TLD6
B	768	GLY	-	expression tag	UNP B3TLD6
B	769	LEU	-	expression tag	UNP B3TLD6
B	770	VAL	-	expression tag	UNP B3TLD6
B	771	PRO	-	expression tag	UNP B3TLD6
B	772	ARG	-	expression tag	UNP B3TLD6
B	773	GLY	-	expression tag	UNP B3TLD6
B	774	SER	-	expression tag	UNP B3TLD6

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

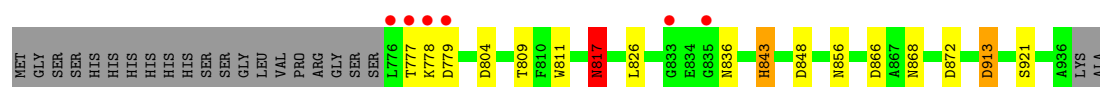
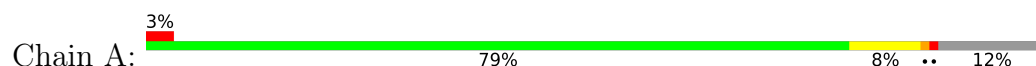
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	61	Total O 61 61	0	0
3	B	75	Total O 75 75	0	0

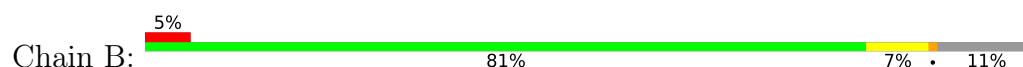
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Lacto-N-biosidase



- Molecule 1: Lacto-N-biosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.78Å 54.78Å 202.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.00 48.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.25-2.00) 100.0 (48.25-2.00)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.224 , 0.240 0.235 , 0.250	Depositor DCC
$R_{free}$ test set	1071 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	0/1245	1.06	4/1710 (0.2%)
1	B	0.59	0/1251	1.08	5/1717 (0.3%)
All	All	0.59	0/2496	1.07	9/3427 (0.3%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	817	ASN	CB-CA-C	6.28	119.58	109.41
1	B	796	HIS	CA-CB-CG	-6.01	107.79	113.80
1	B	925	THR	CA-CB-OG1	-5.71	101.04	109.60
1	A	866	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	792	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	848	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	817	ASN	CB-CA-C	5.16	115.85	108.68
1	A	913	ASP	CB-CA-C	-5.14	98.99	109.94
1	B	920	THR	CA-CB-OG1	-5.05	102.02	109.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1212	0	1149	6	0
1	B	1218	0	1156	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	61	0	0	0	0
3	B	75	0	0	0	0
All	All	2568	0	2305	10	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 2.

All (10) 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:868:ASN:HB2	1:A:872:ASP:OD2	2.04	0.56
1:A:856:ASN:HB2	1:A:913:ASP:HB2	1.89	0.54
1:A:817:ASN:C	1:A:817:ASN:OD1	2.51	0.53
1:B:777:THR:HG23	1:B:778:LYS:H	1.75	0.51
1:A:804:ASP:OD2	1:A:809:THR:OG1	2.29	0.50
1:A:811:TRP:CD2	1:A:826:LEU:HD21	2.48	0.48
1:B:885:PHE:CE1	1:B:894:ILE:HD11	2.49	0.47
1:B:787:ALA:HB2	1:B:826:LEU:HD23	2.02	0.42
1:A:843:HIS:ND1	1:A:843:HIS:C	2.79	0.41
1:B:848:ASP:OD1	1:B:848:ASP:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	159/183 (87%)	152 (96%)	7 (4%)	0	100	100
1	B	160/183 (87%)	154 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	319/366 (87%)	306 (96%)	13 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/142 (87%)	117 (94%)	7 (6%)	17	15
1	B	124/142 (87%)	122 (98%)	2 (2%)	58	64
All	All	248/284 (87%)	239 (96%)	9 (4%)	30	30

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	777	THR
1	A	778	LYS
1	A	779	ASP
1	A	817	ASN
1	A	836	ASN
1	A	843	HIS
1	A	921	SER
1	B	777	THR
1	B	780	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	836	ASN
1	A	851	ASN
1	A	875	ASN
1	A	910	GLN
1	A	912	ASN
1	B	910	GLN

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Mol	Chain	Res	Type
1	B	912	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

### 6.1 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, 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	A	161/183 (87%)	0.08	6 (3%)	45 43	10, 19, 47, 85	0
1	B	162/183 (88%)	-0.09	9 (5%)	31 29	11, 17, 41, 66	0
All	All	323/366 (88%)	-0.01	15 (4%)	38 36	10, 18, 46, 85	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	776	LEU	5.3
1	A	777	THR	5.2
1	B	938	ALA	3.7
1	B	817	ASN	3.2
1	B	796	HIS	3.1
1	A	778	LYS	2.9
1	B	937	LYS	2.6
1	B	778	LYS	2.5
1	B	777	THR	2.5
1	B	835	GLY	2.5
1	B	834	GLU	2.4
1	A	835	GLY	2.2
1	A	779	ASP	2.1
1	A	833	GLY	2.1
1	B	833	GLY	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1001	1/1	0.99	0.01	14,14,14,14	0
2	CA	B	1001	1/1	1.00	0.01	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.