



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 04:36 pm GMT

PDB ID : 2YQ7
Title : Structure of Bcl-xL bound to BimLOCK
Authors : Smith, B.J.; Czabotar, P.E.
Deposited on : 2012-11-06
Resolution : 1.90 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

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**
Xtrriage (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) : 2.36

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 1.90 Å.

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

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.80Å 35.22Å 61.36Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	34.07 – 1.90	Depositor
% Data completeness (in resolution range)	96.7 (34.07-1.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.91Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.208	Depositor
Wilson B-factor (Å ²)	23.6	Xtrriage
Anisotropy	0.040	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1455	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

3 Model quality [i](#)

3.1 Standard geometry [i](#)

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

3.2 Too-close contacts [i](#)

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

3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

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3.3.2 Protein sidechains [i](#)

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

3.3.3 RNA [i](#)

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

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

validation-pack failed to run properly - this section is therefore empty.

3.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

3.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

3.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

3.8 Polymer linkage issues

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

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

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

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

4.3 Carbohydrates

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

4.4 Ligands

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

4.5 Other polymers

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