



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:34 PM EDT

PDB ID : 1BOF / pdb_00001bof
Title : GI-ALPHA-1 BOUND TO GDP AND MAGNESIUM
Authors : Coleman, D.E.; Sprang, S.R.
Deposited on : 1998-08-04
Resolution : 2.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.20 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	I 4	Depositor
Cell constants a, b, c, α , β , γ	121.75Å 121.75Å 68.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	97.3 (15.00-2.20)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.27 (at 2.17Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.227 , 0.268	Depositor
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.143	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
Total number of atoms	2677	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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](#)

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3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

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3.3.2 Protein sidechains [i](#)

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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 ⓘ

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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.