



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:16 PM EDT

PDB ID : 6NS2
Title : Crystal structure of fungal lipoxygenase from *Fusarium graminearum*. P212121 crystal form.
Authors : Pakhomova, S.; Boeglin, W.E.; Neau, D.B.; Bartlett, S.G.; Brash, A.R.; Newcomer, M.E.
Deposited on : 2019-01-24
Resolution : 2.79 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) : 2.35.1

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 2.79 Å.

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

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10158 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 lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	634	5047	3227	838	971	11	0	0	0
1	C	634	5056	3233	842	970	11	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP I1REW2
A	-22	GLY	-	expression tag	UNP I1REW2
A	-21	ARG	-	expression tag	UNP I1REW2
A	-20	ASP	-	expression tag	UNP I1REW2
A	-19	PRO	-	expression tag	UNP I1REW2
A	-18	ASN	-	expression tag	UNP I1REW2
A	-17	SER	-	expression tag	UNP I1REW2
A	-16	SER	-	expression tag	UNP I1REW2
A	-15	SER	-	expression tag	UNP I1REW2
A	-14	VAL	-	expression tag	UNP I1REW2
A	-13	ASP	-	expression tag	UNP I1REW2
A	-12	LYS	-	expression tag	UNP I1REW2
A	-11	LEU	-	expression tag	UNP I1REW2
A	-10	ALA	-	expression tag	UNP I1REW2
A	-9	ALA	-	expression tag	UNP I1REW2
A	-8	ALA	-	expression tag	UNP I1REW2
A	-7	LEU	-	expression tag	UNP I1REW2
A	-6	GLU	-	expression tag	UNP I1REW2
A	-5	HIS	-	expression tag	UNP I1REW2
A	-4	HIS	-	expression tag	UNP I1REW2
A	-3	HIS	-	expression tag	UNP I1REW2
A	-2	HIS	-	expression tag	UNP I1REW2
A	-1	HIS	-	expression tag	UNP I1REW2
A	0	HIS	-	expression tag	UNP I1REW2
C	-23	MET	-	expression tag	UNP I1REW2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	GLY	-	expression tag	UNP I1REW2
C	-21	ARG	-	expression tag	UNP I1REW2
C	-20	ASP	-	expression tag	UNP I1REW2
C	-19	PRO	-	expression tag	UNP I1REW2
C	-18	ASN	-	expression tag	UNP I1REW2
C	-17	SER	-	expression tag	UNP I1REW2
C	-16	SER	-	expression tag	UNP I1REW2
C	-15	SER	-	expression tag	UNP I1REW2
C	-14	VAL	-	expression tag	UNP I1REW2
C	-13	ASP	-	expression tag	UNP I1REW2
C	-12	LYS	-	expression tag	UNP I1REW2
C	-11	LEU	-	expression tag	UNP I1REW2
C	-10	ALA	-	expression tag	UNP I1REW2
C	-9	ALA	-	expression tag	UNP I1REW2
C	-8	ALA	-	expression tag	UNP I1REW2
C	-7	LEU	-	expression tag	UNP I1REW2
C	-6	GLU	-	expression tag	UNP I1REW2
C	-5	HIS	-	expression tag	UNP I1REW2
C	-4	HIS	-	expression tag	UNP I1REW2
C	-3	HIS	-	expression tag	UNP I1REW2
C	-2	HIS	-	expression tag	UNP I1REW2
C	-1	HIS	-	expression tag	UNP I1REW2
C	0	HIS	-	expression tag	UNP I1REW2

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	31	Total O 31 31	0	0
3	C	22	Total O 22 22	0	0

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

3 Data and refinement statistics i

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.49Å 95.06Å 189.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.58 – 2.79	Depositor
% Data completeness (in resolution range)	98.2 (47.58-2.79)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.205 , 0.249	Depositor
Wilson B-factor (Å ²)	46.9	Xtrriage
Anisotropy	1.076	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
Total number of atoms	10158	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.68% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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