



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 10:09 AM UTC

PDB ID : 2IUK / pdb_00002iuk
Title : Crystal structure of Soybean Lipxygenase-D
Authors : Youn, B.; Sellhorn, G.E.; Mirchel, R.J.; Gaffney, B.J.; Grimes, H.D.; Kang, C.
Deposited on : 2006-06-05
Resolution : 2.40 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**
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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 2.40 Å.

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

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13534 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 SEED LIPOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6649	4272	1115	1251	11			
1	B	835	Total	C	N	O	S	0	0	0
			6649	4272	1115	1251	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	PHE	LEU	conflict	UNP P24095
A	233	CYS	SER	conflict	UNP P24095
A	240	LEU	ARG	conflict	UNP P24095
A	364	VAL	TRP	conflict	UNP P24095
A	604	HIS	ASP	conflict	UNP P24095
A	695	LYS	MET	conflict	UNP P24095
B	1192	PHE	LEU	conflict	UNP P24095
B	1233	CYS	SER	conflict	UNP P24095
B	1240	LEU	ARG	conflict	UNP P24095
B	1364	VAL	TRP	conflict	UNP P24095
B	1604	HIS	ASP	conflict	UNP P24095
B	1695	LYS	MET	conflict	UNP P24095

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	113	Total 113	O 113	0	0

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.76Å 115.10Å 120.22Å 90.00° 112.34° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.1 (50.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13534	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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 oligosaccharides 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 [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

5.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

5.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.