



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 06:48 AM 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](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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

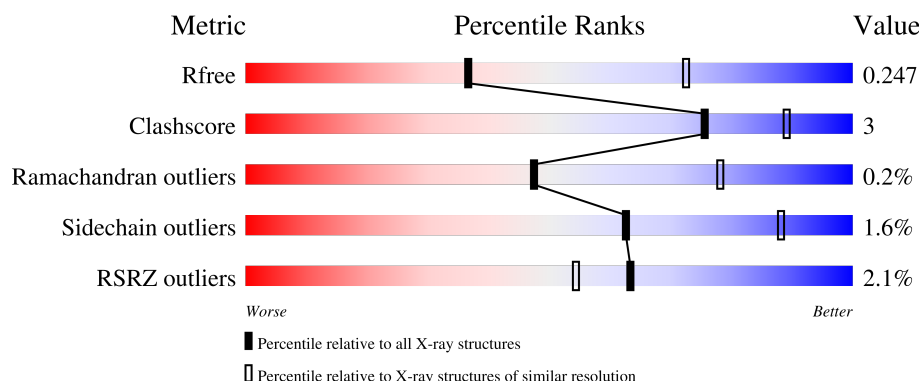
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 Å.

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	769	 75% 8% 18%
1	C	769	 74% 8% 18%

## 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
1	A	634	Total	C	N	O	S	0	0	0
			5047	3227	838	971	11			
1	C	634	Total	C	N	O	S	0	0	0
			5056	3233	842	970	11			

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.49Å 95.06Å 189.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.58 – 2.79 47.53 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.58-2.79) 98.2 (47.53-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.205 , 0.249 0.211 , 0.247	Depositor DCC
$R_{free}$ test set	2019 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	1.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage'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.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.63	0/5174	0.75	1/7036 (0.0%)
1	C	0.64	0/5182	0.74	1/7041 (0.0%)
All	All	0.64	0/10356	0.74	2/14077 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	ASN	CB-CA-C	-7.78	94.84	110.40
1	C	496	TYR	CB-CG-CD1	5.19	124.11	121.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5047	0	4919	29	0
1	C	5056	0	4956	32	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	31	0	0	0	0
3	C	22	0	0	0	0
All	All	10158	0	9875	61	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 3.

All (61) 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:C:695:ASN:ND2	1:C:698:THR:OG1	2.18	0.77
1:A:504:ARG:NH2	1:A:519:TYR:OH	2.25	0.68
1:C:504:ARG:NH2	1:C:519:TYR:OH	2.28	0.67
1:A:539:VAL:O	1:A:542:SER:HB3	2.00	0.61
1:C:539:VAL:O	1:C:542:SER:HB3	2.00	0.60
1:A:504:ARG:HH22	1:A:519:TYR:HH	1.50	0.58
1:C:658:LEU:HB3	1:C:659:PRO:HD3	1.84	0.58
1:A:402:HIS:HE1	1:A:603:GLN:HE21	1.52	0.56
1:C:597:THR:HG21	1:C:739:THR:HA	1.88	0.55
1:A:658:LEU:HB3	1:A:659:PRO:HD3	1.88	0.55
1:A:597:THR:HG21	1:A:739:THR:HA	1.88	0.54
1:C:593:SER:HB3	1:C:594:PRO:CD	2.37	0.54
1:A:554:PRO:HG2	1:A:555:TYR:CE2	2.44	0.53
1:A:593:SER:HB3	1:A:594:PRO:CD	2.38	0.53
1:C:554:PRO:HG2	1:C:555:TYR:CE2	2.44	0.53
1:C:402:HIS:HE1	1:C:603:GLN:HE21	1.55	0.52
1:C:435:ILE:HD12	1:C:585:VAL:HG11	1.91	0.52
1:A:408:LEU:O	1:A:412:HIS:HB2	2.09	0.51
1:A:435:ILE:HD12	1:A:585:VAL:HG11	1.94	0.50
1:C:454:LEU:O	1:C:458:VAL:HB	2.12	0.50
1:C:408:LEU:O	1:C:412:HIS:HB2	2.13	0.48
1:C:437:SER:N	1:C:438:PRO:CD	2.77	0.48
1:C:593:SER:HB3	1:C:594:PRO:HD3	1.95	0.47
1:A:454:LEU:O	1:A:458:VAL:HB	2.14	0.47
1:A:412:HIS:CE1	1:A:446:LEU:HD21	2.48	0.47
1:C:412:HIS:CE1	1:C:446:LEU:HD21	2.49	0.47
1:A:385:TRP:N	1:A:386:PRO:CD	2.78	0.47
1:A:593:SER:HB3	1:A:594:PRO:HD3	1.96	0.47
1:A:265:LYS:O	1:A:269:TYR:HD2	1.98	0.46
1:A:437:SER:N	1:A:438:PRO:CD	2.78	0.46
1:C:280:LYS:HB3	1:C:371:LEU:CD1	2.46	0.46
1:C:385:TRP:N	1:C:386:PRO:CD	2.78	0.46
1:A:455:VAL:HB	1:A:456:PRO:HD3	1.97	0.46
1:A:166:GLU:OE2	1:A:657:GLN:NE2	2.44	0.46
1:C:166:GLU:OE2	1:C:657:GLN:NE2	2.44	0.46
1:C:265:LYS:O	1:C:269:TYR:HD2	1.98	0.45
1:C:455:VAL:HB	1:C:456:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:VAL:HG11	1:C:482:LEU:HD23	1.99	0.45
1:A:177:VAL:HG21	1:A:318:LEU:HD12	1.98	0.45
1:A:280:LYS:HB3	1:A:371:LEU:CD1	2.47	0.44
1:C:300:ARG:HD3	1:C:307:ASN:HD22	1.82	0.44
1:A:300:ARG:HD3	1:A:307:ASN:HD22	1.81	0.44
1:A:677:LYS:HD3	1:A:707:TYR:CE1	2.53	0.44
1:C:437:SER:HA	1:C:440:TRP:CE3	2.53	0.44
1:C:478:ASN:HD22	1:C:481:LYS:HD2	1.83	0.43
1:C:370:ARG:NH1	1:C:375:ASP:O	2.51	0.43
1:A:404:VAL:HG11	1:A:482:LEU:HD23	1.99	0.43
1:C:177:VAL:HG21	1:C:318:LEU:HD12	2.01	0.43
1:C:504:ARG:HH22	1:C:519:TYR:HH	1.58	0.43
1:A:478:ASN:HD22	1:A:481:LYS:HD2	1.83	0.42
1:A:590:HIS:CE1	1:A:595:GLN:HB2	2.55	0.42
1:A:610:VAL:N	1:A:611:PRO:CD	2.82	0.42
1:C:610:VAL:N	1:C:611:PRO:CD	2.83	0.42
1:A:437:SER:HA	1:A:440:TRP:CE3	2.55	0.42
1:C:496:TYR:CE2	1:C:583:ASP:HB3	2.55	0.42
1:C:439:HIS:CD2	1:C:589:ILE:HG12	2.54	0.41
1:A:187:HIS:HB2	1:A:190:THR:HG23	2.02	0.41
1:C:590:HIS:CE1	1:C:595:GLN:HB2	2.55	0.41
1:C:340:GLN:HB2	1:C:350:LEU:HD11	2.02	0.41
1:A:730:GLU:HG3	1:A:732:PRO:HD3	2.03	0.40
1:C:423:ASN:ND2	1:C:433:TYR:OH	2.46	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	630/769 (82%)	601 (95%)	28 (4%)	1 (0%)	47 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	630/769 (82%)	599 (95%)	30 (5%)	1 (0%)	47 78
All	All	1260/1538 (82%)	1200 (95%)	58 (5%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	SER
1	C	593	SER

### 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	541/660 (82%)	533 (98%)	8 (2%)	65 89
1	C	544/660 (82%)	535 (98%)	9 (2%)	60 87
All	All	1085/1320 (82%)	1068 (98%)	17 (2%)	62 88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	ASP
1	A	188	GLU
1	A	200	VAL
1	A	274	GLN
1	A	289	LYS
1	A	519	TYR
1	A	543	GLN
1	A	738	THR
1	C	184	ASP
1	C	200	VAL
1	C	210	LYS
1	C	274	GLN
1	C	287	ASP
1	C	376	THR

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Mol	Chain	Res	Type
1	C	519	TYR
1	C	543	GLN
1	C	579	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	307	ASN
1	A	309	GLN
1	A	362	ASN
1	A	478	ASN
1	A	568	GLN
1	A	580	GLN
1	A	590	HIS
1	A	595	GLN
1	A	603	GLN
1	A	671	ASN
1	A	685	ASN
1	C	294	GLN
1	C	307	ASN
1	C	309	GLN
1	C	423	ASN
1	C	478	ASN
1	C	568	GLN
1	C	580	GLN
1	C	590	HIS
1	C	595	GLN
1	C	603	GLN
1	C	685	ASN
1	C	695	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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

### 6.1 Protein, DNA and RNA chains

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	634/769 (82%)	0.15	10 (1%) 72 66	34, 55, 83, 130	0
1	C	634/769 (82%)	0.32	17 (2%) 54 44	32, 66, 108, 125	0
All	All	1268/1538 (82%)	0.23	27 (2%) 63 54	32, 58, 101, 130	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	266	ILE	5.7
1	C	100	GLY	4.7
1	C	628	LEU	4.2
1	A	100	GLY	3.9
1	C	270	ILE	3.7
1	C	636	LEU	3.5
1	A	378	ASP	3.5
1	C	186	ASP	3.4
1	C	185	ILE	3.2
1	C	378	ASP	3.0
1	A	286	GLU	2.8
1	C	379	ILE	2.6
1	C	634	LYS	2.5
1	C	210	LYS	2.5
1	A	697	LYS	2.4
1	A	645	GLU	2.4
1	C	383	GLU	2.4
1	A	374	ASP	2.3
1	C	102	GLU	2.3
1	C	116	ARG	2.2
1	C	645	GLU	2.2
1	A	634	LYS	2.2
1	A	540	ILE	2.1
1	A	188	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	365	THR	2.1
1	C	134	ASP	2.1
1	A	287	ASP	2.0

## 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 monosaccharides 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	FE2	A	801	1/1	0.93	0.20	43,43,43,43	0
2	FE2	C	801	1/1	0.94	0.11	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.