



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 10:32 PM EDT

PDB ID : 6NLF  
Title : 1.45 Å resolution structure of apo BfrB from *Pseudomonas aeruginosa*  
Authors : Lovell, S.; Punchi-Hewage, A.; Battaile, K.P.; Yao, H.; Nammalwar, B.;  
Gnanasekaran, K.K.; Bunce, R.A.; Reitz, A.B.; Rivera, M.  
Deposited on : 2019-01-08  
Resolution : 1.45 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>.

---

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 1.45 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 18267 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 Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1324	836	224	256	8	0	7	0
1	B	156	1307	826	219	254	8	0	6	0
1	C	156	1312	828	221	255	8	0	6	0
1	D	156	1315	831	222	254	8	0	6	0
1	E	156	1307	826	219	254	8	0	6	0
1	F	156	1316	831	220	257	8	0	7	0
1	G	156	1328	838	225	257	8	0	8	0
1	H	156	1315	830	222	255	8	0	6	0
1	I	156	1318	832	223	255	8	0	6	0
1	J	156	1327	838	225	256	8	0	7	0
1	K	156	1324	837	224	255	8	0	7	0
1	L	156	1323	836	223	256	8	0	7	0

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total K 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	203	Total O 203 203	0	0
3	B	197	Total O 197 197	0	0
3	C	211	Total O 211 211	0	0
3	D	203	Total O 203 203	0	0
3	E	213	Total O 213 213	0	0
3	F	201	Total O 201 201	0	0
3	G	184	Total O 184 184	0	0
3	H	192	Total O 192 192	0	0
3	I	214	Total O 214 214	0	0
3	J	223	Total O 223 223	0	0
3	K	191	Total O 191 191	0	0
3	L	216	Total O 216 216	0	0

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

### 3 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.73Å 197.77Å 204.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.18 – 1.45	Depositor
% Data completeness (in resolution range)	99.9 (37.18-1.45)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 1.45Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.147 , 0.165	Depositor
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtrriage
Anisotropy	0.206	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	18267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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.

## 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 3 ligands modelled in this entry, 3 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 failed to run properly - this section is therefore empty.

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

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

### 5.3 Carbohydrates [i](#)

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

### 5.4 Ligands [i](#)

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

### 5.5 Other polymers [i](#)

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