



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 12:07 am BST

PDB ID : 1FR1  
Title : REFINED CRYSTAL STRUCTURE OF BETA-LACTAMASE FROM CITROBACTER FREUNDII INDICATES A MECHANISM FOR BETA-LACTAM HYDROLYSIS  
Authors : Oefner, C.; D'Arcy, A.; Daly, J.J.; Winkler, F.K.  
Deposited on : 2000-09-07  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.11

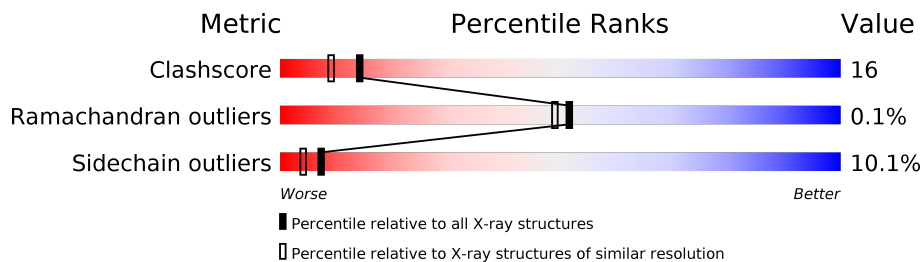
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 on 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	
1	B	361	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6057 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 BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2799	1796	477	517	9	0	0	0
1	B	361	2806	1801	479	517	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	SER	THR	SEE REMARK 999	UNP Q46041
A	176	LYS	THR	SEE REMARK 999	UNP Q46041
A	180	HIS	GLN	SEE REMARK 999	UNP Q46041
A	228	ILE	VAL	SEE REMARK 999	UNP Q46041
A	253	GLU	LYS	SEE REMARK 999	UNP Q46041
A	278	VAL	LEU	SEE REMARK 999	UNP Q46041
A	285	SER	ASN	SEE REMARK 999	UNP Q46041
A	348	VAL	ALA	SEE REMARK 999	UNP Q46041
B	175	SER	THR	SEE REMARK 999	UNP Q46041
B	176	LYS	THR	SEE REMARK 999	UNP Q46041
B	180	HIS	GLN	SEE REMARK 999	UNP Q46041
B	228	ILE	VAL	SEE REMARK 999	UNP Q46041
B	253	GLU	LYS	SEE REMARK 999	UNP Q46041
B	278	VAL	LEU	SEE REMARK 999	UNP Q46041
B	285	SER	ASN	SEE REMARK 999	UNP Q46041
B	348	VAL	ALA	SEE REMARK 999	UNP Q46041

- Molecule 2 is water.

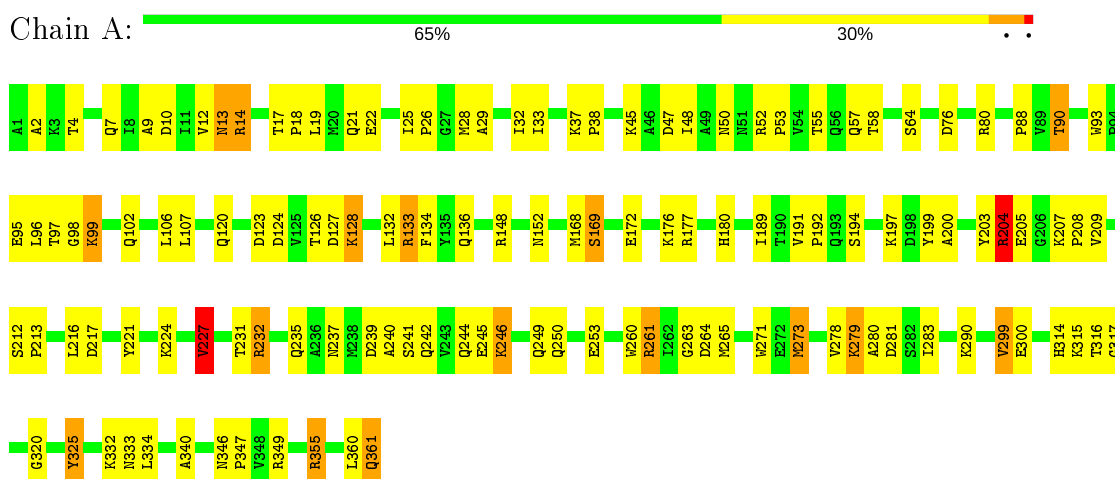
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	211	Total	O	0	0
			211	211		
2	B	241	Total	O	0	0
			241	241		

### 3 Residue-property plots

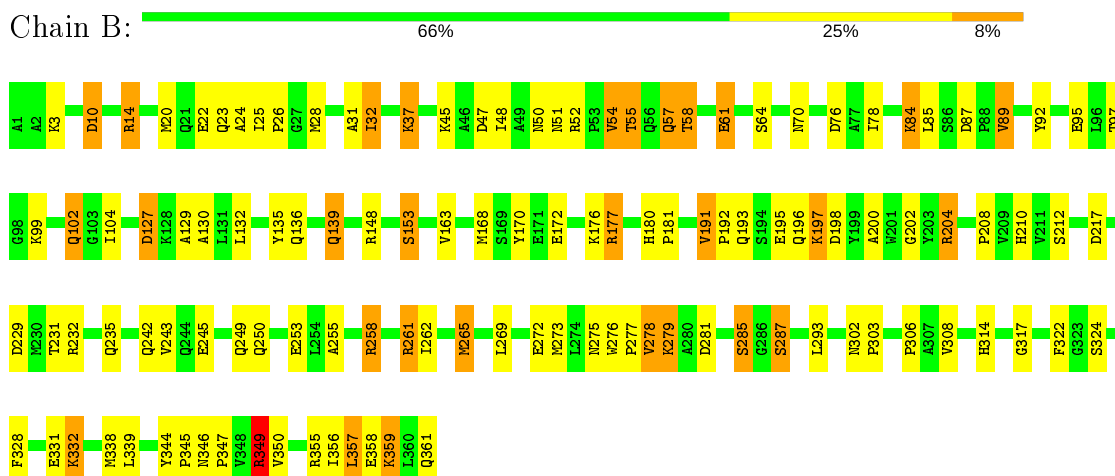
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: BETA-LACTAMASE



- Molecule 1: BETA-LACTAMASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.07Å 84.63Å 89.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	87.0 (6.00-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality [i](#)

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

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	1.04	2/2874 (0.1%)	1.51	25/3918 (0.6%)
1	B	1.10	4/2881 (0.1%)	1.63	32/3925 (0.8%)
All	All	1.07	6/5755 (0.1%)	1.57	57/7843 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	GLU	CD-OE1	-6.77	1.18	1.25
1	B	355	ARG	CD-NE	-6.17	1.35	1.46
1	B	278	VAL	N-CA	-5.60	1.35	1.46
1	A	278	VAL	N-CA	-5.53	1.35	1.46
1	A	227	VAL	CB-CG2	5.37	1.64	1.52

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ARG	CD-NE-CZ	21.10	153.14	123.60
1	B	349	ARG	NE-CZ-NH1	19.52	130.06	120.30
1	A	273	MET	CA-CB-CG	16.61	141.53	113.30
1	B	355	ARG	NE-CZ-NH1	16.36	128.48	120.30
1	B	349	ARG	CD-NE-CZ	12.24	140.74	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	349	ARG	Sidechain

## 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	2799	0	2776	89	7
1	B	2806	0	2796	90	12
2	A	211	0	0	18	18
2	B	241	0	0	9	26
All	All	6057	0	5572	174	34

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 16.

The worst 5 of 174 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:A:361:GLN:CA	2:A:503:HOH:O	1.86	1.24
1:A:361:GLN:C	2:A:503:HOH:O	1.84	1.13
1:A:227:VAL:HG23	2:A:417:HOH:O	1.51	1.10
1:B:55:THR:H	1:B:58:THR:CG2	1.78	0.96
1:A:55:THR:HG22	1:A:57:GLN:H	1.35	0.88

The worst 5 of 34 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:507:HOH:O	2:B:529:HOH:O[2_664]	0.07	2.13
2:A:511:HOH:O	2:B:553:HOH:O[2_664]	0.17	2.03
2:B:436:HOH:O	2:B:477:HOH:O[2_665]	0.34	1.86
2:A:561:HOH:O	2:B:596:HOH:O[4_455]	0.36	1.84

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:508:HOH:O	2:B:549:HOH:O[3_645]	0.39	1.81

## 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	359/361 (99%)	350 (98%)	8 (2%)	1 (0%)	41 37
1	B	359/361 (99%)	345 (96%)	14 (4%)	0	100 100
All	All	718/722 (99%)	695 (97%)	22 (3%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	GLY

### 5.3.2 Protein sidechains [i](#)

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	290/292 (99%)	260 (90%)	30 (10%)	7 4
1	B	292/292 (100%)	263 (90%)	29 (10%)	8 4
All	All	582/584 (100%)	523 (90%)	59 (10%)	7 4

5 of 59 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	299	VAL
1	B	45	LYS
1	B	314	HIS
1	A	314	HIS
1	A	361	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	B	91	GLN
1	B	302	ASN
1	B	50	ASN
1	B	56	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.