



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 09:40 pm BST

PDB ID : 1IWG  
Title : Crystal structure of Bacterial Multidrug Efflux transporter AcrB  
Authors : Murakami, S.; Nakashima, R.; Yamashita, E.; Yamaguchi, A.  
Deposited on : 2002-05-15  
Resolution : 3.50 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
Xtriage (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

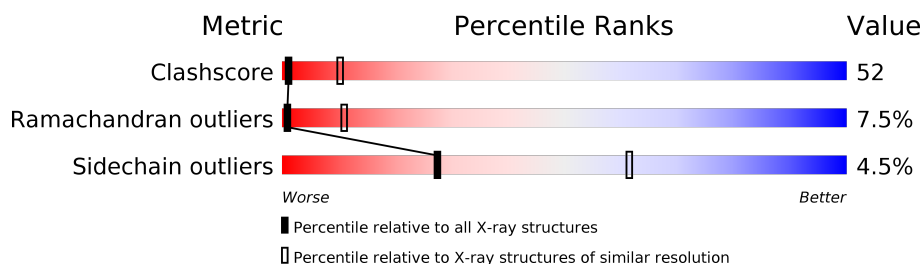
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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	1053	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7639 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 AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1006	Total	C	N	O	S	0	0	0
			7639	4916	1262	1419	42			

There are 4 discrepancies between the modelled and reference sequences:

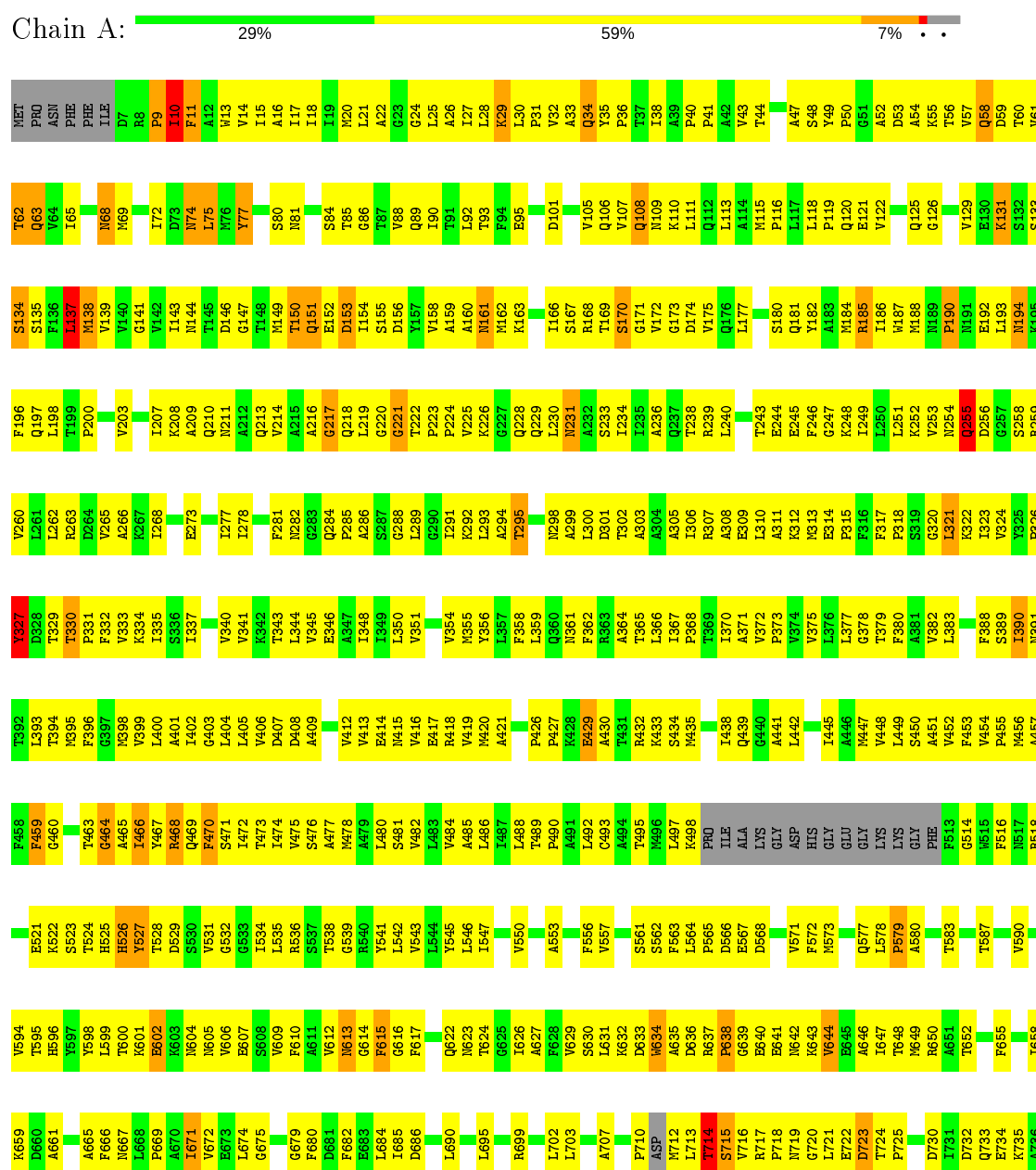
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224

### 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: AcrB



Q737	P804	A878	I943	X1008
A738	S805	I879	L944	G1009
L739	S806	S880	I945	G1010
G740		L881	Y946	M1011
V741	S813	I882	E947	V1012
S742	P814	V883	F948	T1013
I743	R815	V884	A949	A1014
I744	L816	F885	K950	T1015
D745	E817	L886	D951	
	R818	C887	L952	V1016
	Y819	L888	K953	L1017
		A889	D954	A1018
		A890	K955	I1019
	P823	A891	F956	F1020
A752	S824	L892	E957	F1021
A753	M825	Y892	K958	V1022
M754	E826	E893		P1023
	I827	S894	G959	V1024
Y758	L828	W895	L960	F1025
V759	G829	S896	I961	F1026
I760	Q830	I897		F1027
D761	A831	P898	T964	V1028
F762	P832	F899	L965	V1029
I763	P833	S900	D966	R1030
D764	G834	V901	A967	R1031
	K835	M902	V968	R1032
	S836	L903	R969	F1033
	I837	V904	P970	S1034
R767		V905	R971	R1035
V768	K769	P906	L972	K1036
K770	E842	P907	R973	ASN
V771	L843	I907	P974	GLU
V772	M844	G968	I975	ASP
V773	E845	V909	L976	ILE
M774	Q846	I910	V977	GLU
S775	L847	G911	T978	HIS
E776	A912	L913	S979	SER
A777	L851	L914	L980	HIS
K778	P852	A915	A981	THR
Y779				VAL
R780	V855	R919	F982	ASP
M781	D858	G920	L983	HIS
L782	W859	L921	L984	HIS
P783	THR	T922	G985	HIS
	GLY	N923	V986	HIS
I786	MET	D924	V987	HIS
	SER	Y925	P988	HIS
W789	TYR	V926	L989	HIS
Y790	GLN	F927	V990	
V791	ARG	I991	S992	
R792	LEU	S997		
A793		G998	A999	
A794	S869			
D795	G870	L932		A1002
G796	N871	T933		V1003
Q797	Q872			G1004
V799	A873	L937		T1005
P800	P874	S938		G1006
F801	S875	A939		V1007
S802	L876	R940		
A803	Y877	N941		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.54Å 144.54Å 519.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.290 , 0.355	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	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	0.27	0/7779	0.51	3/10563 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	949	ALA	C-N-CA	-11.25	93.58	121.70
1	A	949	ALA	CA-C-N	5.73	129.80	117.20
1	A	950	LYS	CB-CA-C	5.27	120.95	110.40

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	7639	0	7800	805	1
All	All	7639	0	7800	805	1

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 52.

The worst 5 of 805 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:598:TYR:HB3	1:A:606:VAL:HG21	1.39	1.05
1:A:108:GLN:HB3	1:A:129:VAL:HG11	1.42	0.99
1:A:151:GLN:HB3	1:A:285:PRO:HB3	1.45	0.97
1:A:240:LEU:HD12	1:A:245:GLU:HB3	1.42	0.97
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.46	0.96

All (1) 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)
1:A:525:HIS:NE2	1:A:525:HIS:NE2[4_556]	2.10	0.10

## 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	998/1053 (95%)	725 (73%)	198 (20%)	75 (8%)	<b>1</b> <b>11</b>

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	10	ILE
1	A	29	LYS
1	A	134	SER
1	A	146	ASP

### 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	818/859 (95%)	781 (96%)	37 (4%)	27	61

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	A	613	ASN
1	A	1023	PRO
1	A	429	GLU
1	A	439	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	360	GLN
1	A	797	GLN
1	A	255	GLN
1	A	391	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.