



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:21 PM GMT

PDB ID : 1T9U  
Title : Structural Basis of Multidrug Transport by the AcrB Multidrug Efflux Pump  
Authors : Yu, E.W.; McDermott, G.; Nikaido, H.  
Deposited on : 2004-05-18  
Resolution : 3.11 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

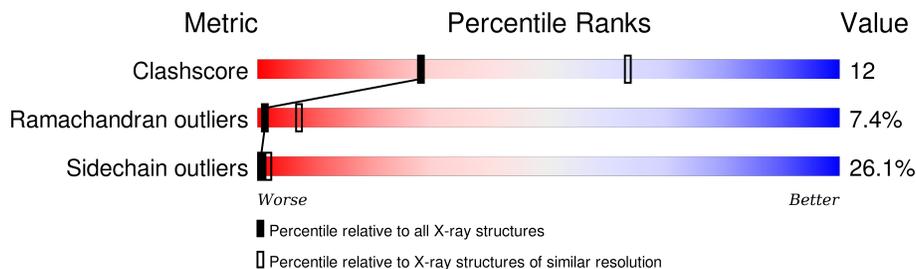
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1049	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CPF	A	5002	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7739 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.

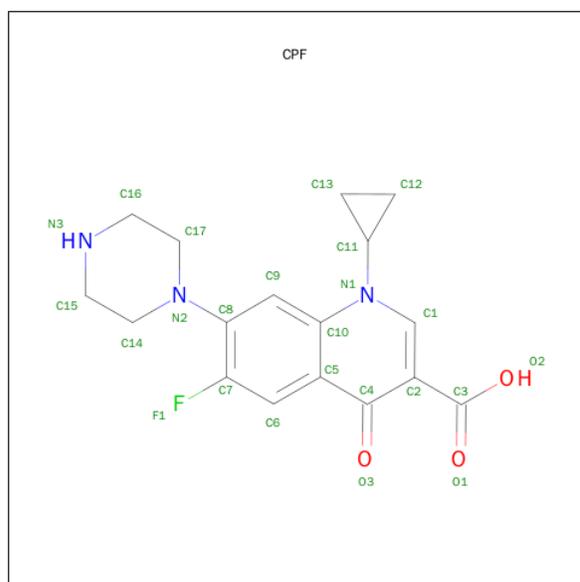
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1013	7691	4946	1272	1431	42	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	ASN	ENGINEERED	UNP P31224

- Molecule 2 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (three-letter code: CPF) (formula:  $C_{17}H_{18}FN_3O_3$ ).



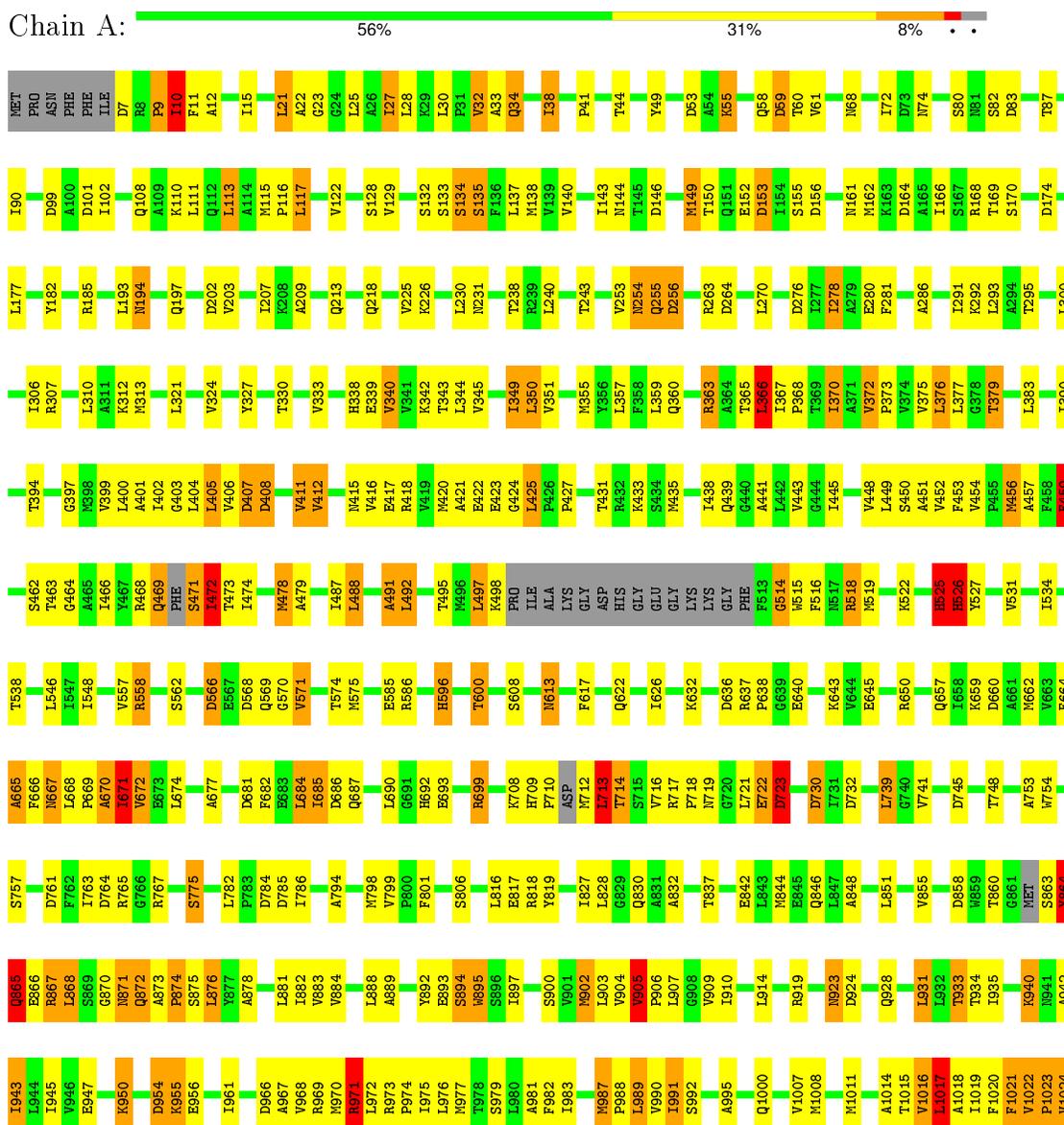
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	24	17	1	3	3	0	0
2	A	1	24	17	1	3	3	0	0

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Acriflavine resistance protein B



F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	ILE	GLU	HIS	SER	HIS	THR	VAL	ASP	HIS	HIS
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## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.09Å 144.09Å 518.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	182.57 – 3.11	Depositor
% Data completeness (in resolution range)	(Not available) (182.57-3.11)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.265 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

## 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: CPF

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	0.36	0/7830	0.73	35/10630 (0.3%)

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	2	4

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1032	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	722	GLU	N-CA-C	6.12	127.53	111.00
1	A	568	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	924	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	966	ASP	CB-CG-OD2	5.77	123.49	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	722	GLU	CA
1	A	954	ASP	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	525	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	A	712	MET	Peptide
1	A	864	TYR	Peptide
1	A	867	ARG	Peptide

## 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	7691	0	7851	181	0
2	A	48	0	34	10	0
All	All	7739	0	7885	181	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 12.

The worst 5 of 181 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:830:GLN:NE2	2:A:5002:CPF:H121	1.53	1.22
1:A:830:GLN:HE22	2:A:5002:CPF:C12	1.59	1.09
1:A:667:ASN:OD1	2:A:5002:CPF:H152	1.53	1.06
1:A:830:GLN:HE22	2:A:5002:CPF:H121	0.80	0.96
1:A:667:ASN:OD1	2:A:5002:CPF:C15	2.19	0.90

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	1003/1049 (96%)	795 (79%)	134 (13%)	74 (7%)	<b>1</b> <b>7</b>

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	22	ALA
1	A	34	GLN
1	A	134	SER
1	A	135	SER

### 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	823/854 (96%)	608 (74%)	215 (26%)	<b>0</b> <b>2</b>

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	SER
1	A	608	SER
1	A	977	MET
1	A	478	MET
1	A	557	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN
1	A	605	ASN
1	A	1000	GLN
1	A	577	GLN
1	A	613	ASN

### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CPF	A	5001	-	21,27,27	0.95	1 (4%)	28,40,40	1.14	2 (7%)
2	CPF	A	5002	1	21,27,27	0.94	1 (4%)	28,40,40	1.14	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPF	A	5001	-	-	0/4/22/22	0/3/4/4
2	CPF	A	5002	1	-	0/4/22/22	0/3/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	CPF	C4-C5	3.38	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5002	CPF	C4-C5	3.39	1.45	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	CPF	C2-C4-C5	-3.46	116.00	121.87
2	A	5002	CPF	C2-C4-C5	-3.43	116.04	121.87
2	A	5002	CPF	C4-C5-C10	2.82	121.30	118.54
2	A	5001	CPF	C4-C5-C10	2.83	121.30	118.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5002	CPF	10	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.