



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 1IWG / pdb_00001iwg
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

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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

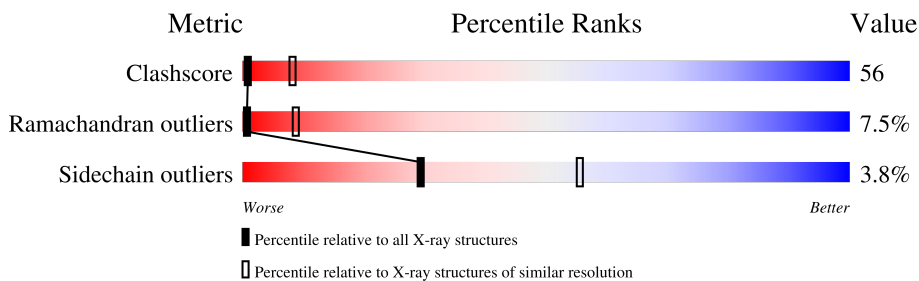
1 Overall quality at a glance

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	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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 ≥ 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	 28% 60% 7% . .

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:

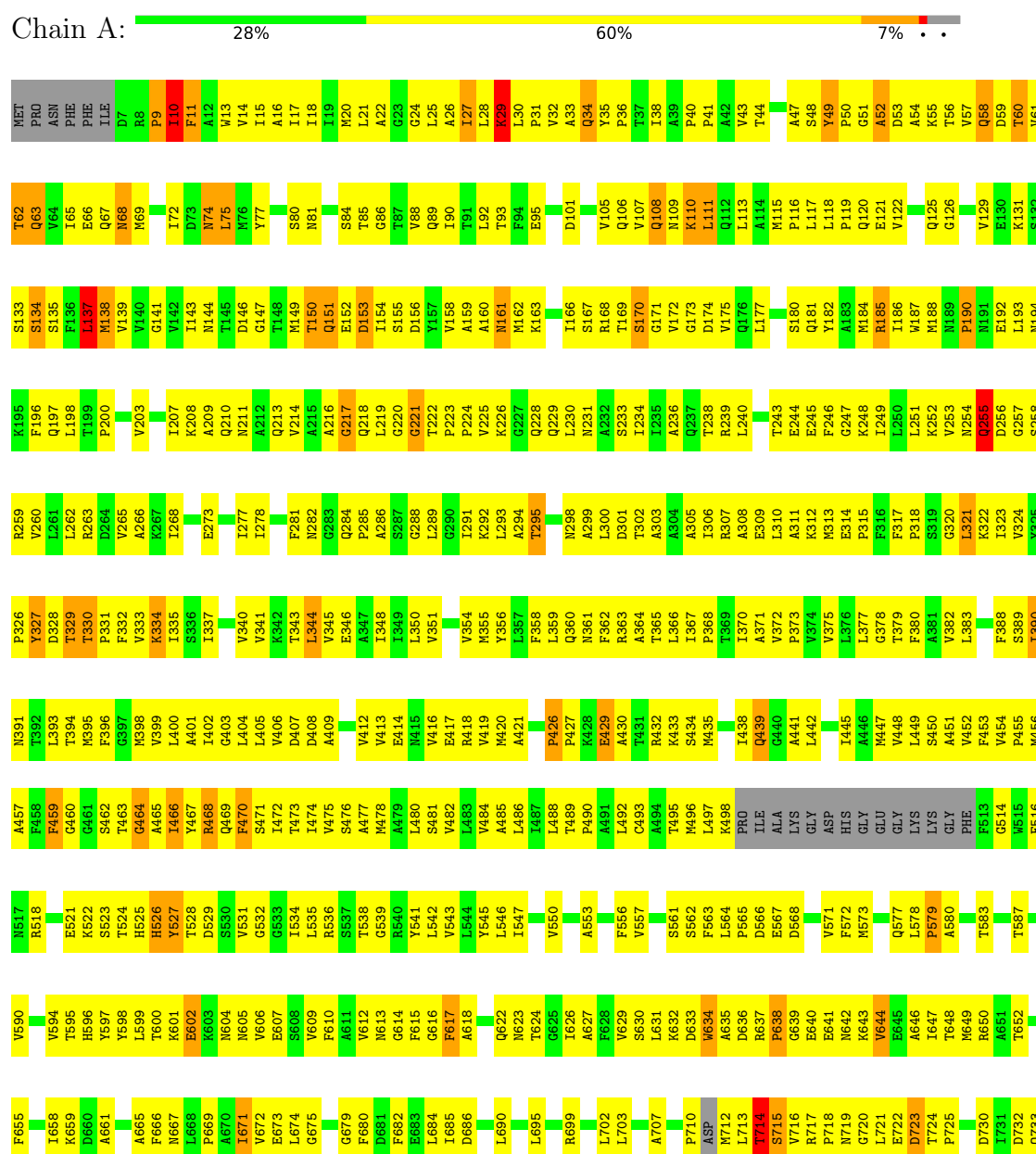
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



V1003	G1004	T1005	G1006	V1007	M1008	G1009	G1010	M1011	V1012	T1013	A1014	T1015	V1016	L1017	A1018	T1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	ILE	GLU	HIS	SER	HIS	HIS	THR	VAL	ASP	HIS	HIS	HIS	HIS	HIS																
S938	A939	K940	N941	A942	I943	L944	I945	V946	E947	F948	A949	K950	D951	L952	M953	D954	K955	E956	G957	K958	G959	L960	I961		T964	L965	D966	A967	V968	R969	M970	R971	L972	R973	P974	I975	L976	M977	T978	S979	L980	A981	F982	I983	L984	G985	V986	M987	P988	L989	V990	I991	S992		S997	G998	A999		A1002							
E734	K735	A736	Q737	L738	A739	G740	V741	S742	I743	N744	D745			T748	T749	L750	G751	A752	M753	M754		Y758	V759	N760	D761	F762	I763	D764	R765	G766	G767	V768	K769	K770	V771	Y772	V773	M774	S775	E776	A777	K778	Y779	R780	M781	L782	P783		I786		W789	Y790	V791	R792	A793	M794	D795	G796	Q797	M798						
V799	P800	F801	S802	A803	F804	S805	S806		S813	P814	R815	L816	E817	R818	Y819		P823	S824	M825	E826	I827	L828	G829	Q830		A831	A832	P833	G834	K835	S836	T837		E842	L843	M844	E845	Q846	L847		L851	A852		V855		D858	W859		THR	GLY	MET	SER	TYR	GLN	R792	ARG	A793	I794	D795	G796	Q797	N871	S869	G870	N871	Q872
A873	P874	S875	L876	Y877	A878	I879	S880	L881	I882	V883	V884	F885	L886	C887	L888	A889	A890	L891	Y892	E893	S894	W895	S896	I897	P898	F899	S900	V901	M902	L903	V904	V905	P906	L907	G908	V909	I910	G911	A912	L913	L914	A915		R919	G920	L921	W859		T922	N923	D924	V925	F926	F927	Q928	V929		L932	T933		L937					

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, α , β , γ	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 ²)	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	0.31	1/7779 (0.0%)	0.84	16/10563 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	949	ALA	N-CA	-6.35	1.37	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	949	ALA	CA-C-N	-15.75	93.58	121.14
1	A	949	ALA	C-N-CA	-15.75	93.58	121.14
1	A	110	LYS	N-CA-C	-8.57	102.95	113.41
1	A	844	MET	N-CA-C	-6.07	105.79	113.43
1	A	49	TYR	CA-C-N	6.01	127.35	119.84

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	861	1
All	All	7639	0	7800	861	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 56.

The worst 5 of 861 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%)	1 9

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%)	787 (96%)	31 (4%)	29 55

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	LEU
1	A	895	TRP
1	A	439	GLN
1	A	1023	PRO
1	A	815	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	760	ASN
1	A	797	GLN
1	A	923	ASN
1	A	228	GLN
1	A	213	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.