



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (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

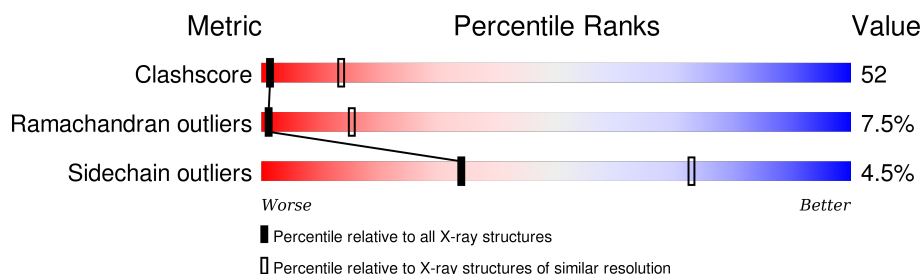
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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 ≥ 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	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:

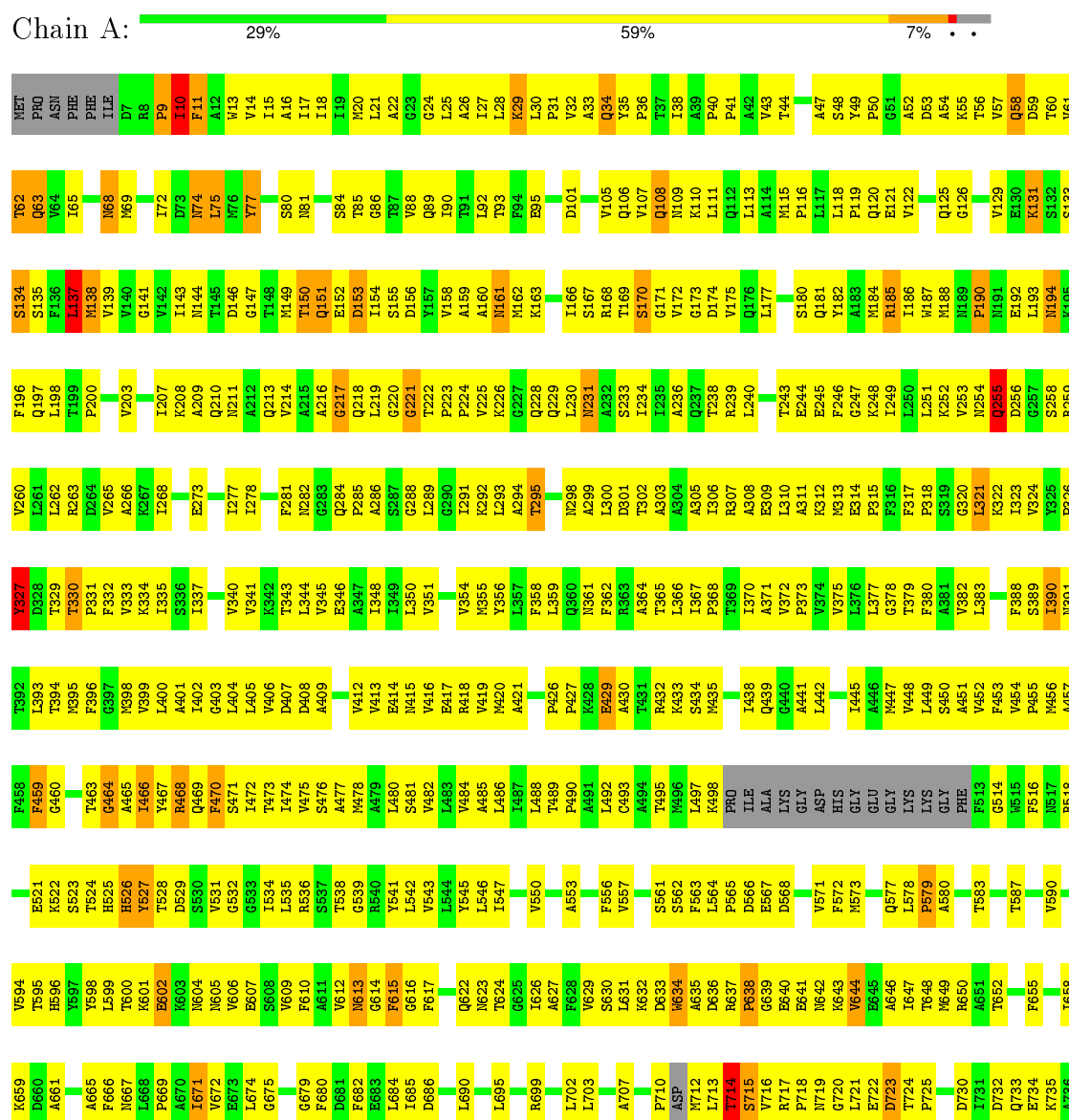
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224

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 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: AcrB



V1008	Q737	P804	A878	I943
G1009	A738	S805	L879	L944
G1010	L739	S806	S880	L945
M1011	G740		L881	Y946
V1012	V741	S813	V882	E947
A1013	S742	P814	V883	T1013
A1014	L743	R815	V884	A1014
T1015	D744	L816	F885	A949
V1016	D745	E817	L886	K950
L1017		R818	C887	D951
A1018	T748	X819	L888	L952
I1019	T749		L889	Y953
F1020		P823	A890	D954
F1021	A752	S824	V891	V955
V1022	A753	M825	L891	E956
V1023	W754	E826	Y892	G957
V1024		I827	E893	K958
F1025	Y758	L828	S894	G959
F1026	V759	G829	N895	L960
V1027	D761	Q830	S896	I961
V1028	F762	A831	L897	T964
Y1029	F763	P832	P898	L965
R1030	L764	P833	F899	L966
R1031		G834	S900	D966
R1032		K835	Y901	A967
F1033		S836	N902	V968
S1034		T837	L903	R969
R1035			Y904	Y970
K1036			V905	R971
ASN	R767	E842	P906	L972
GLU	V768	L843	L907	R973
ASP	K769	M844	G908	P974
ILE	V770	E845	V909	L975
GLU	V771	Q846	L910	L976
HIS	V772	L847	G911	Y977
SER	V773		A912	T978
HIS	S775		L913	Y979
HIS	E776	L851	L914	L980
THR	A777	P852	A915	L981
VAL	V778			A982
ASP	V779	V855	R919	P983
HIS	A780	D858	G920	L984
HIS	L782	W859	L921	G985
HIS	P783	THR	T922	V986
HIS		GLY	D923	V987
HIS	I786	MET	D924	P988
HIS		SER	V925	L989
		TYR	Y926	Y990
		GLN	F927	I991
		ARG	Q928	S992
		LEU	V929	
		S869	L932	S997
		G870	T933	G998
		Q797		A999
		N871	L937	A1002
		Q872	S938	V1003
		A873	A939	G1004
		P874	R940	T1005
		S875	N941	G1006
		L876	A942	V1007
		Y877		

4 Data and refinement statistics

Xtriage (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, 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	0.27	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%)	1	15

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%)	34 73

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 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.