



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:42 pm GMT

PDB ID : 2I6W
Title : Crystal structure of the multidrug efflux transporter AcrB
Authors : Das, D.; Xu, Q.S.; Kim, S.H.
Deposited on : 2006-08-29
Resolution : 3.10 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

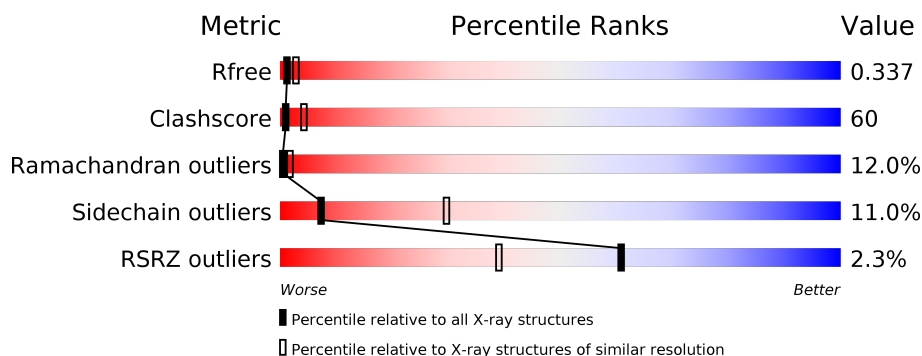
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	1049	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7737 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.

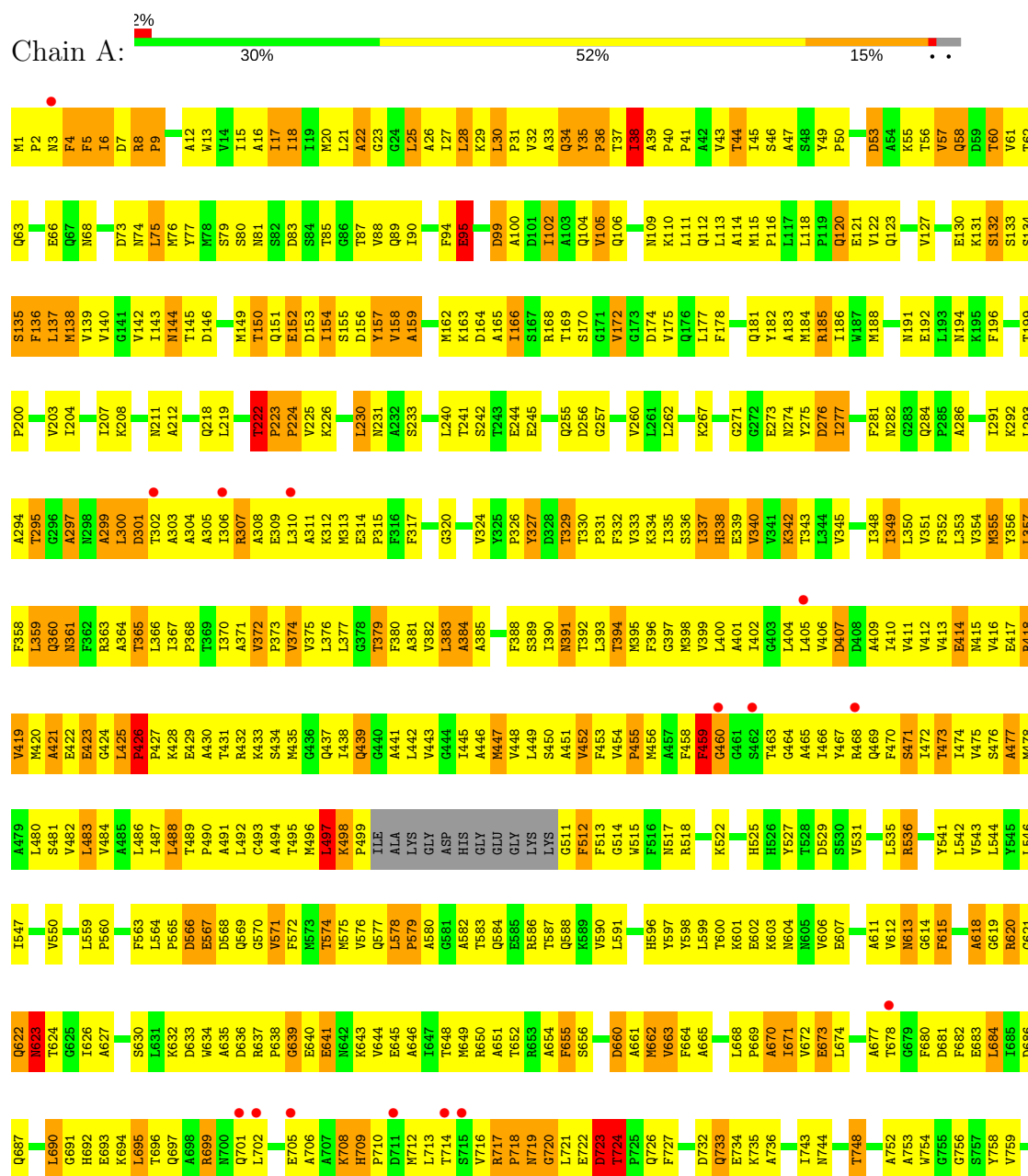
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1019	7737	4983	1270	1440	44	0	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 the various outlier classes 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.

• Molecule 1: Acriflavine resistance protein B



F1026	F762	Q830	E893	L960	F762	Q830	E893	L960	F1026
V1027	I763	A831	S894	I961	A831	S894	S894	I961	V1027
V1028	D764	A832	W895	T964	A832	W895	S896	T964	V1028
V1029	R765	P833	S896	L965	P833	S896	I897	L965	V1029
R1030	G766	K834	I897	D966	K834	I897	P898	D966	R1030
ARG	R767	K835	P898	A967	K835	P898	F899	A967	ARG
ARG	W768	S836	F899	V968	S836	F899	S900	V968	ARG
PHE	K769	T837	S900	R969	T837	S900	V901	R969	PHE
SER	K770	G838	V901	P970	G838	V901	M902	P970	SER
ARG	M774	E839	M902	R971	E839	M902	L903	R971	ARG
LYS	S775	A840	L903	L972	A840	L903	M903	L972	LYS
ASN		W841	M903	R973	W841	M903	L904	R973	ASN
GLU		E842	L904	P974	E842	L904	V905	P974	GLU
ASP		L843	P906	I975	L843	P906	L907	I975	ASP
ASP		M844	L907	L976	M844	L907	G908	L976	ASP
ILE		E845	G908	M977	E845	G908	V909	M977	ILE
GLU		Q846	V909	T978	Q846	V909	I910	T978	GLU
HIS		L847	I910	S979	L847	I910	G911	S979	HIS
SER		L851	G911	L980	L851	G911	L914	L980	SER
HIS		D784	L914	A981	D784	L914	T917	A981	HIS
THR		D785	T917	F982	D785	T917	F918	F982	THR
VAL		I786	F918	L983	I786	F918	L984	L983	VAL
ASP			L984	L985		L984	G985	L985	ASP
HIS			G985	V986		G985	V986	M987	HIS
HIS			V986	M987		V986	P988	P988	HIS
			M987	P988		M987	L989	L989	
			P988	L989		P988	V990	V990	
			L989	V990		L989	I991	I991	
			V990	I991		V990	S992	S992	
			I991	S992		I991	T993	T993	
			S992	T993		S992	G994	G994	
			T993	G994		T993	A995	A995	
			G994	A995		G994	G996	G996	
			A995	G996		A995	S997	S997	
			G996	S997		G996	G998	G998	
			S997	G998		S997	A999	A999	
			G998	A999		G998	Q1000	Q1000	
			A999	Q1000		A999	N1001	N1001	
			Q1000	N1001		Q1000	A1002	A1002	
			N1001	A1002		N1001	V1003	V1003	
			A1002	V1003		A1002	G1004	G1004	
			V1003	G1004		V1003	T1005	T1005	
			G1004	T1005		G1004	G1006	G1006	
			T1005	G1006		T1005	V1007	V1007	
			G1006	V1007		G1006	M1008	M1008	
			V1007	M1008		V1007	G1009	G1009	
			M1008	G1009		M1008	V1016	V1016	
			G1009	V1016		G1009	L1017	L1017	
			V1016	L1017		V1016	A1018	A1018	
			L1017	A1018		L1017	I1019	I1019	
			A1018	I1019		A1018	F1020	F1020	
			I1019	F1020		I1019	F1021	F1021	
			F1020	F1021		F1020	V1022	V1022	
			F1021	V1022		F1021	P1023	P1023	
			V1022	P1023		V1022	V1024	V1024	
			P1023	V1024		P1023	F1025	F1025	
			V1024	F1025		V1024			
			F1025			F1025			

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	146.30Å 146.30Å 514.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.12 – 3.10 45.12 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.12-3.10) 99.7 (45.12-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.305 , 0.341 0.300 , 0.337	Depositor DCC
R_{free} test set	1952 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7737	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.46	0/7884	0.74	5/10712 (0.0%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ARG	N-CA-C	-6.93	92.29	111.00
1	A	497	LEU	N-CA-C	6.33	128.08	111.00
1	A	972	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	497	LEU	CA-CB-CG	-5.17	103.40	115.30
1	A	300	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	TYR	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	7737	0	7884	934	3
All	All	7737	0	7884	934	3

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 60.

The worst 5 of 934 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:104:GLN:HG3	1:A:131:LYS:HG3	1.19	1.14
1:A:472:ILE:HD12	1:A:473:THR:H	1.11	1.11
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.30	1.10
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.23	1.08
1:A:363:ARG:HB3	1:A:497:LEU:HD13	1.35	1.06

All (3) 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:529:ASP:OD1	1:A:529:ASP:OD1[11_445]	1.93	0.27
1:A:529:ASP:OD2	1:A:529:ASP:OD2[11_445]	2.12	0.08
1:A:525:HIS:NE2	1:A:529:ASP:OD2[11_445]	2.18	0.02

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	1015/1049 (97%)	688 (68%)	205 (20%)	122 (12%)	0 2

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	6	ILE
1	A	17	ILE
1	A	38	ILE
1	A	132	SER

5.3.2 Protein sidechains ⓘ

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	829/855 (97%)	738 (89%)	91 (11%)	7 30

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	ARG
1	A	604	ASN
1	A	958	LYS
1	A	426	PRO
1	A	483	LEU

Some 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	210	GLN
1	A	284	GLN
1	A	871	ASN
1	A	213	GLN
1	A	231	ASN

5.3.3 RNA ⓘ

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1019/1049 (97%)	-0.14	23 (2%) 61 39	23, 66, 111, 160	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ILE	4.0
1	A	714	THR	3.9
1	A	678	THR	3.4
1	A	833	PRO	3.3
1	A	702	LEU	2.9

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.