



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2023 – 02:18 AM EDT

PDB ID : 2HQD  
Title : Conformation of the AcrB Multidrug Efflux Pump in Mutants of the Putative Proton Relay Pathway  
Authors : Su, C.-C.; Li, M.; Gu, R.; Takatsuka, Y.; McDermott, G.; Nikaido, H.; Yu, E.W.  
Deposited on : 2006-07-18  
Resolution : 3.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

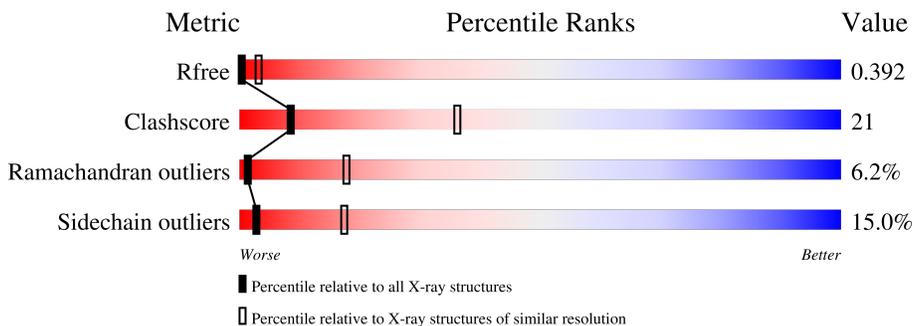
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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))
$R_{free}$	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)

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  $\geq 3$ , 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  $\leq 5\%$ .

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 7718 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	1016	7718	4964	1276	1435	43	0	0	0

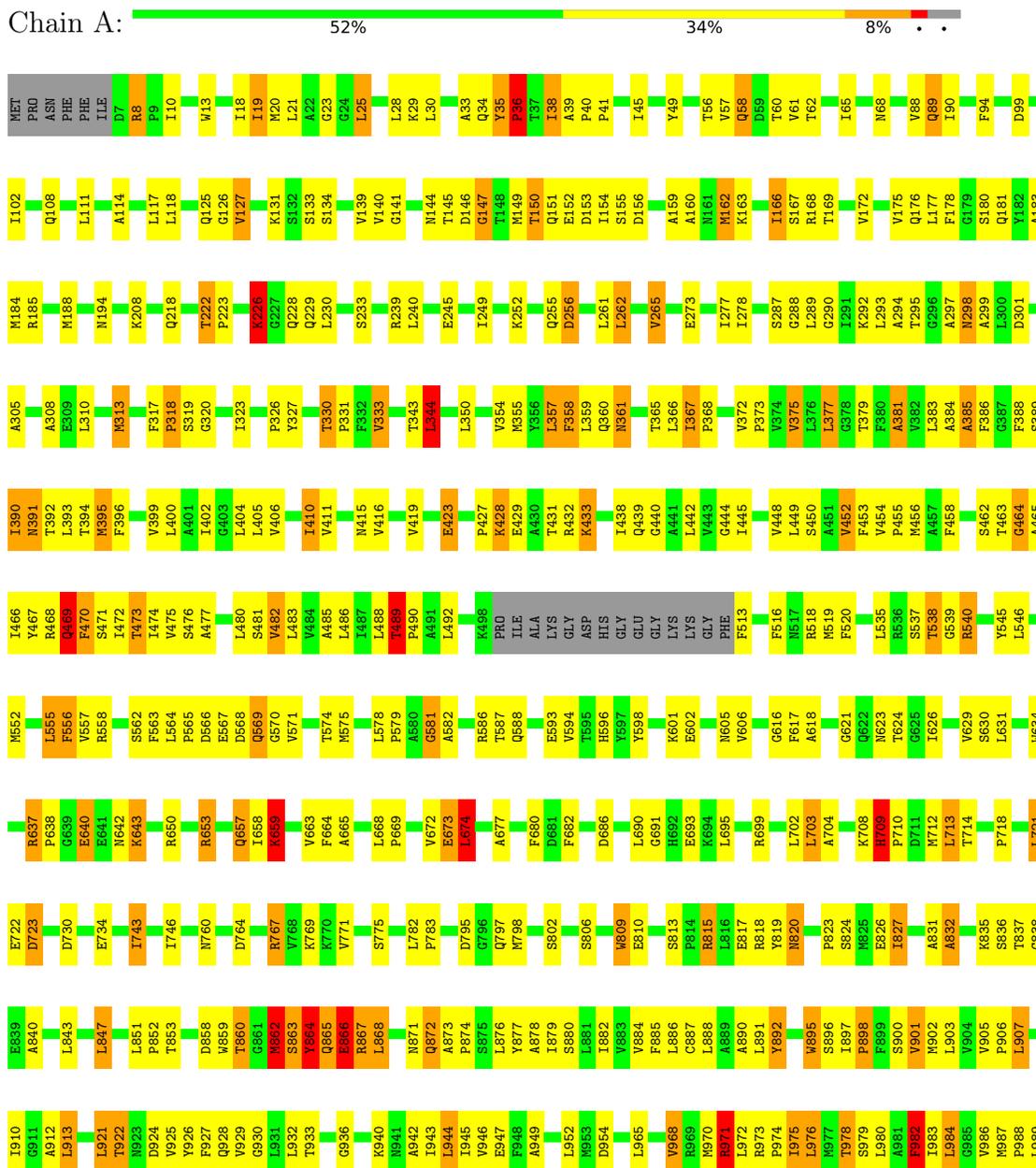
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	ALA	ASP	engineered mutation	UNP P31224
A	1050	HIS	-	cloning artifact	UNP P31224
A	1051	HIS	-	cloning artifact	UNP P31224
A	1052	HIS	-	cloning artifact	UNP P31224
A	1053	HIS	-	cloning artifact	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.

- Molecule 1: Acriflavine resistance protein B



T990	T991	S992	T993	Q1000	N1001	A1002	V1003	V1007	M1008	G1009	G1010	M1011	V1012	T1013	A1014	T1015	A1018	I1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	R1031	R1032	F1033	S1034	R1035	R1036	ASN	GLU	ASP	ASP	ILE	GLU	HIS	SER	HIS	HIS	THR	VAL	ASP	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.03Å 145.03Å 513.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.65 46.68 – 3.65	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-3.65) 89.7 (46.68-3.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.76 (at 3.66Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.261 , 0.303 0.369 , 0.392	Depositor DCC
$R_{free}$ test set	1101 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.4	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	7718	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.83	23/7861 (0.3%)	0.74	10/10676 (0.1%)

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	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	LYS	CD-CE	15.58	1.90	1.51
1	A	1031	ARG	NE-CZ	15.31	1.52	1.33
1	A	1035	ARG	CZ-NH1	14.66	1.52	1.33
1	A	1031	ARG	CZ-NH1	13.14	1.50	1.33
1	A	256	ASP	C-O	12.44	1.47	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1031	ARG	NE-CZ-NH2	-24.13	108.24	120.30
1	A	35	TYR	C-N-CD	-16.10	85.18	120.60
1	A	1035	ARG	NE-CZ-NH2	-13.84	113.38	120.30
1	A	35	TYR	C-N-CA	10.04	164.15	122.00
1	A	1031	ARG	NE-CZ-NH1	7.26	123.93	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1031	ARG	Sidechain
1	A	469	GLN	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	7718	0	7878	325	0
All	All	7718	0	7878	325	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 21.

The worst 5 of 325 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:433:LYS:CE	1:A:433:LYS:CD	1.90	1.46
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.11	1.08
1:A:926:TYR:HB3	1:A:1003:VAL:HG23	1.31	1.07
1:A:1022:VAL:HB	1:A:1023:PRO:CD	1.83	1.07
1:A:653:ARG:O	1:A:657:GLN:HB2	1.61	0.99

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	1012/1053 (96%)	770 (76%)	179 (18%)	63 (6%)	<b>1</b> <b>18</b>

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	PRO
1	A	150	THR
1	A	166	ILE
1	A	167	SER
1	A	358	PHE

### 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	826/858 (96%)	702 (85%)	124 (15%)	<b>3</b> <b>17</b>

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	520	PHE
1	A	952	LEU
1	A	637	ARG
1	A	944	LEU
1	A	991	ILE

Sometimes 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	604	ASN
1	A	657	GLN
1	A	622	GLN
1	A	687	GLN
1	A	151	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 monosaccharides 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

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.