

wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 09:00 AM EDT

PDB ID	:	10YD
Title	:	Structural Basis of Multiple Binding Capacity of the AcrB multidrug Efflux
		Pump
Authors	:	Yu, E.W.; MeDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on	:	2003-04-03
Resolution	:	3.80 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 (i) 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 (1)) were used in the production of this report:

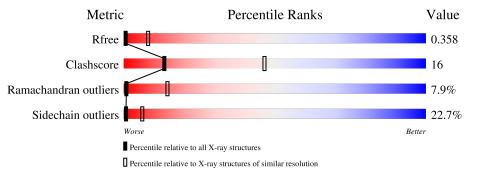
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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 <=5%

Mol	Chain	Length	Quality of chain			
1	А	1049	54%	33%	8% • •	

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	DEQ	А	4001	-	Х	-	-



2 Entry composition (i)

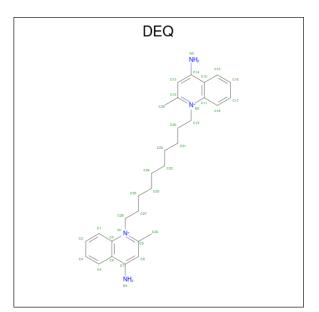
There are 2 unique types of molecules in this entry. The entry contains 7673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	
1	А	1006	Total 7639	C 4916	N 1262	O 1419	S 42	0	0	0

• Molecule 2 is DEQUALINIUM (three-letter code: DEQ) (formula: $C_{30}H_{40}N_4$).

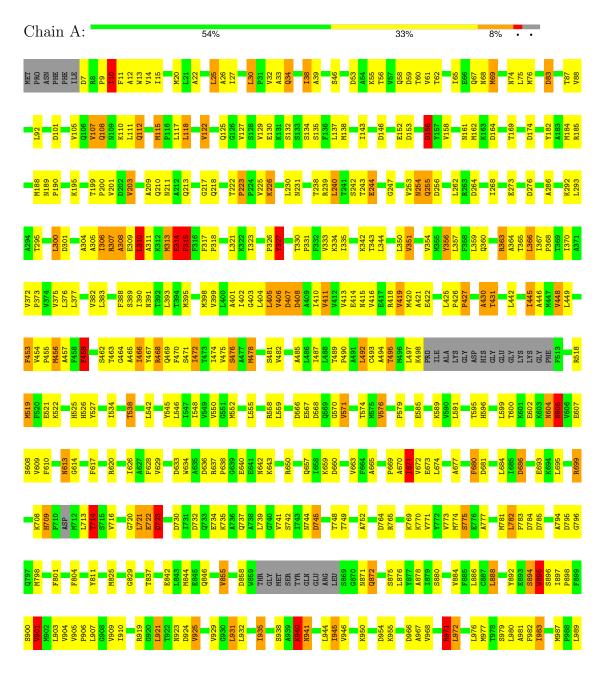


Ν	Iol	Chain	Residues	Atoms			ZeroOcc	AltConf
	2	А	1	Total 34	C 30	N 4	0	0



3 Residue-property plots (i)

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



V000 V000 1991 5992 5993 7993 7994 7993 7002 1008 71015 71015 71015 71015 71015 71015 71015 71015 71015 71015 71015 71015 71016 71015 71017 71015 71018 71016 71019 71016 71016 71016 71017 71016 71018 71016 71019 71016 71016 71016 71017 71016 71018 71016 71019 71016 71026 71026 71027 71026 71036 71036 611 71036 612 71036 613 612 614 71036 614 71036 615 71036</td



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	144.77Å 144.77Å 517.89Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 - 3.80	Depositor
Resolution (A)	46.61 - 3.78	EDS
% Data completeness	$100.0 \ (46.60-3.80)$	Depositor
(in resolution range)	$99.4 \ (46.61 - 3.78)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.66 (at 3.77 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.0	Depositor
D D.	0.284 , 0.338	Depositor
R, R_{free}	0.362 , 0.358	DCC
R_{free} test set	1083 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	156.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26, 92.3	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms $(Å^2)$	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: DEQ

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).

Mal	Chain	Bond	lengths	Bond angles		
IVIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.36	0/7779	0.75	35/10563~(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	А	2	0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	310	LEU	CA-CB-CG	9.04	136.09	115.30
1	А	315	PRO	N-CA-C	6.82	129.84	112.10
1	А	795	ASP	CB-CG-OD2	6.40	124.06	118.30
1	А	568	ASP	CB-CG-OD2	6.31	123.98	118.30
1	А	407	ASP	CB-CG-OD2	6.13	123.82	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	А	470	PHE	CA
1	А	680	PHE	CA

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	А	7639	0	7800	229	1
2	А	34	0	36	20	0
All	All	7673	0	7836	249	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 16.

The worst 5 of 249 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)
2:A:4001:DEQ:C20	2:A:4001:DEQ:C21	1.80	1.57
2:A:4001:DEQ:C22	2:A:4001:DEQ:C23	1.83	1.52
2:A:4001:DEQ:C27	2:A:4001:DEQ:C28	1.84	1.51
1:A:313:MET:C	1:A:315:PRO:HD3	1.82	0.99
2:A:4001:DEQ:C20	2:A:4001:DEQ:C22	2.51	0.89

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:226:LYS:O	1:A:596:HIS:NE2[16_445]	1.90	0.30

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	Analysed Favoured		Outliers	Percentiles	
1	А	998/1049~(95%)	759 (76%)	160 (16%)	79~(8%)	1 14	

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	9	PRO
1	А	10	ILE
1	А	34	GLN
1	А	135	SER
1	А	255	GLN

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	А	818/855~(96%)	632~(77%)	186 (23%)	1 6

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	620	ARG
1	А	798	MET
1	А	643	LYS
1	А	709	HIS
1	А	855	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	667	ASN
1	А	941	ASN
1	А	228	GLN
1	А	284	GLN
1	А	391	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	Mol Type Cha	Type	Chain	Chain Res		Res	Link	B	ond leng	gths	E	ond ang	gles
WIOI		Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2			
2	DEQ	А	4001	-	35,37,37	4.96	17 (48%)	46,50,50	3.90	28 (60%)			

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	DEQ	А	4001	-	-	9/13/13/13	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
2	А	4001	DEQ	C11-N2	14.85	1.58	1.40
2	А	4001	DEQ	C12-N2	12.63	1.53	1.36
2	А	4001	DEQ	C5-N1	12.36	1.55	1.40

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
2	А	4001	DEQ	C27-C28	9.03	1.84	1.51
2	А	4001	DEQ	C9-N1	7.68	1.46	1.36

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	4001	DEQ	C12-N2-C11	-12.08	111.53	122.12
2	А	4001	DEQ	C19-N2-C11	10.63	133.07	118.98
2	А	4001	DEQ	C21-C20-C19	7.97	140.76	112.25
2	А	4001	DEQ	C20-C19-N2	-5.94	98.51	111.83
2	А	4001	DEQ	C25-C24-C23	5.90	144.18	114.37

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	4001	DEQ	C27-C28-N1-C5
2	А	4001	DEQ	C27-C28-N1-C9
2	А	4001	DEQ	C20-C19-N2-C11
2	А	4001	DEQ	C20-C19-N2-C12
2	А	4001	DEQ	C26-C27-C28-N1

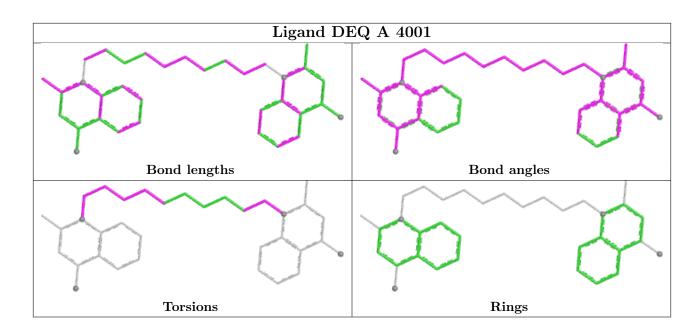
There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	4001	DEQ	20	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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)

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

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

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

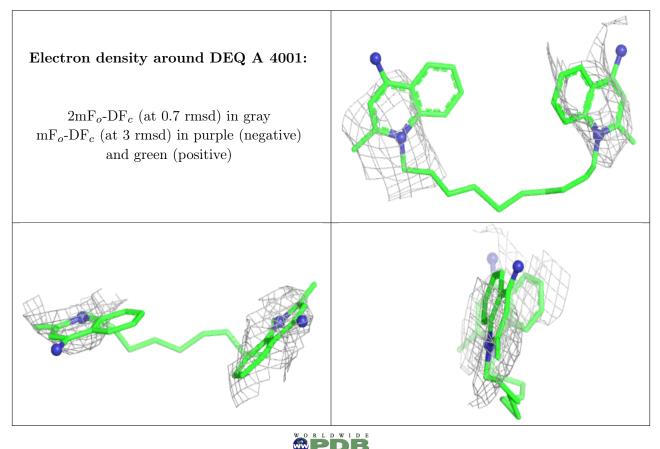
6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

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

