



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:16 AM GMT

PDB ID : 2GFP  
Title : Structure of the Multidrug Transporter EmrD from Escherichia coli  
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Deposited on : 2006-03-22  
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](mailto: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.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

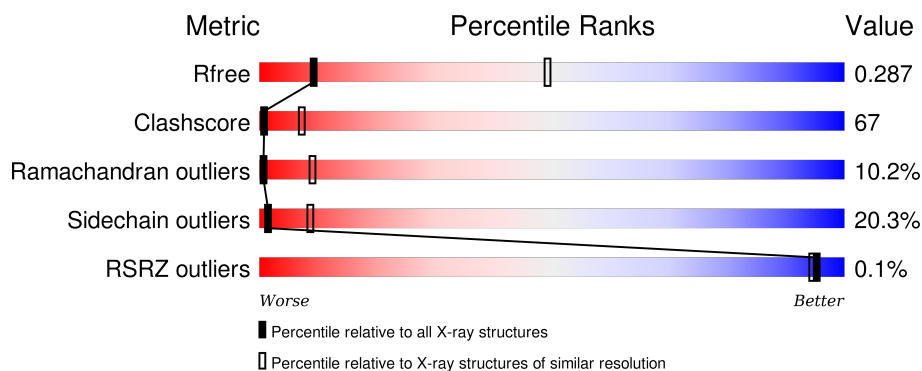
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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  $\geq 3$ , 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	375	 25% 53% 18% .
1	B	375	 25% 53% 18% .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5600 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.

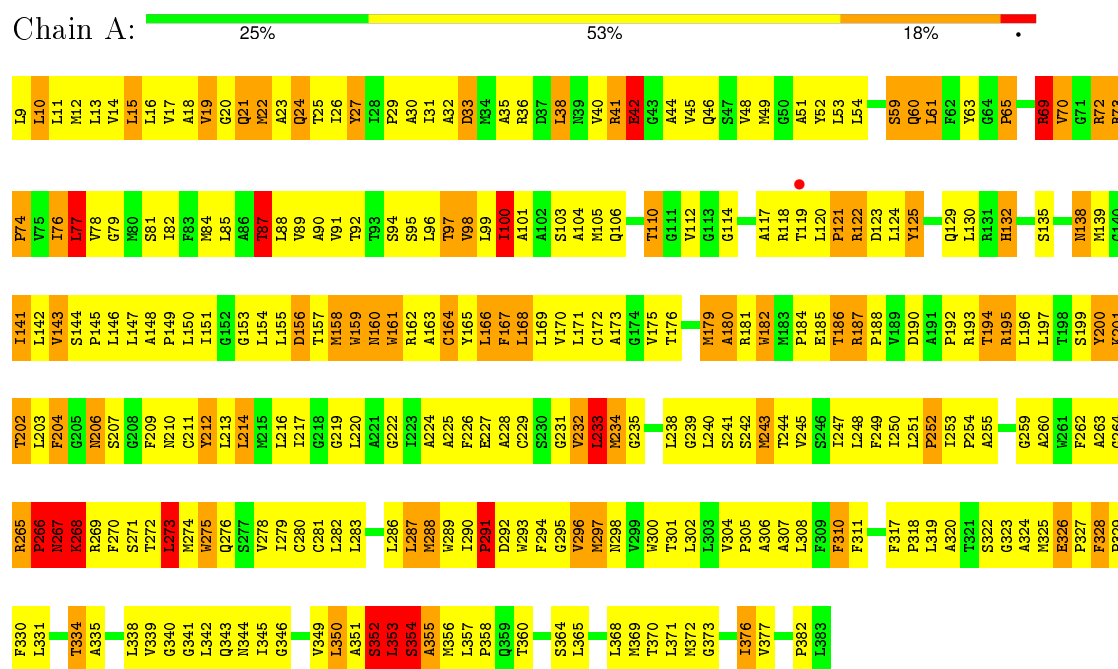
- Molecule 1 is a protein called Multidrug resistance protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2800	1842	455	472	31			
1	B	375	Total	C	N	O	S	0	0	0
			2800	1842	455	472	31			

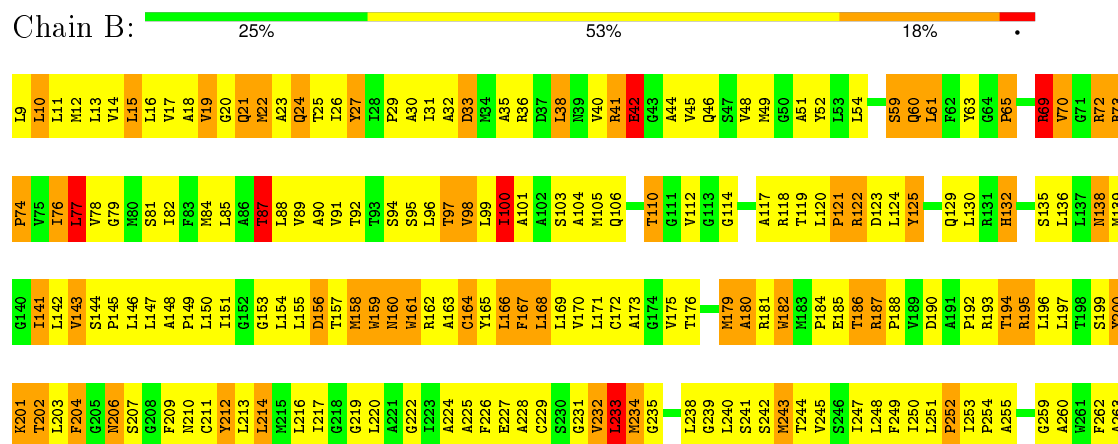
### 3 Residue-property plots

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.

#### • Molecule 1: Multidrug resistance protein D



#### • Molecule 1: Multidrug resistance protein D



Q264	P329
R265	F330
P266	L331
I267	
K268	T334
R269	A335
F270	
S271	
T272	
L273	L338
M274	V339
M275	G340
Q276	G341
S277	L342
V278	Q343
I279	M344
C280	I345
C281	G346
L282	
L283	V349
	L350
	A351
L286	S352
L287	L353
M288	S354
M289	A355
T290	M356
P291	L357
D292	P358
M293	Q359
F294	T360
G295	
V296	S364
M297	L365
M298	
V299	L368
M300	M369
T301	T370
L302	L371
L303	M372
V304	G373
P305	
A306	I376
A307	V377
L308	
F309	P382
F310	L383
F311	
	F317
	P318
	L319
	A320
	T321
	S322
	G323
	A324
	M325
	E326
	P327
	F328

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.50 Å   124.50 Å   109.40 Å 90.00°   110.20°   90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.01 – 3.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.50) 61.7 (50.01-3.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.39 (at 3.48 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.270   ,   0.350 0.229   ,   0.287	Depositor DCC
$R_{free}$ test set	1321 reflections (9.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	87.1	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.03 , 5.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 13426 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.38	0/2864	0.84	15/3900 (0.4%)
1	B	0.38	0/2864	0.84	15/3900 (0.4%)
All	All	0.38	0/5728	0.84	30/7800 (0.4%)

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	1	2
1	B	1	2
All	All	2	4

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	LEU	C-N-CA	8.44	142.81	121.70
1	A	353	LEU	C-N-CA	8.40	142.70	121.70
1	B	77	LEU	CA-CB-CG	6.87	131.11	115.30
1	A	77	LEU	CA-CB-CG	6.84	131.04	115.30
1	A	352	SER	N-CA-C	6.49	128.53	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	233	LEU	CA
1	B	233	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	LEU	Mainchain
1	A	354	SER	Mainchain
1	B	353	LEU	Mainchain
1	B	354	SER	Mainchain

## 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	2800	0	2932	392	0
1	B	2800	0	2932	389	0
All	All	5600	0	5864	767	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 67.

The worst 5 of 767 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:200:TYR:HE1	1:B:204:PHE:CE1	1.38	1.40
1:A:200:TYR:CE1	1:B:204:PHE:CE1	2.29	1.21
1:A:263:ALA:HA	1:A:268:LYS:HB2	1.15	1.10
1:B:20:GLY:HA2	1:B:110:THR:HB	1.32	1.09
1:A:20:GLY:HA2	1:A:110:THR:HB	1.32	1.08

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	373/375 (100%)	268 (72%)	67 (18%)	38 (10%)	1	9
1	B	373/375 (100%)	268 (72%)	67 (18%)	38 (10%)	1	9
All	All	746/750 (100%)	536 (72%)	134 (18%)	76 (10%)	1	9

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	69	ARG
1	A	87	THR
1	A	97	THR
1	A	180	ALA

### 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	295/295 (100%)	235 (80%)	60 (20%)	1	9
1	B	295/295 (100%)	235 (80%)	60 (20%)	1	9
All	All	590/590 (100%)	470 (80%)	120 (20%)	1	9

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	PHE
1	B	41	ARG
1	B	287	LEU
1	A	334	THR
1	B	10	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN

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Mol	Chain	Res	Type
1	B	298	ASN
1	B	106	GLN
1	A	206	ASN
1	B	60	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	375/375 (100%)	-0.82	1 (0%) 94 91	80, 80, 80, 80	0
1	B	375/375 (100%)	-0.79	0 100 100	80, 80, 80, 80	0
All	All	750/750 (100%)	-0.80	1 (0%) 95 94	80, 80, 80, 80	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	THR	2.3

### 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.