



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:26 am BST

PDB ID : 5Y50  
Title : Crystal structure of eukaryotic MATE transporter AtDTX14  
Authors : Miyauchi, H.; Kusakizako, T.; Nishizawa, T.; Ishitani, R.; Nureki, O.  
Deposited on : 2017-08-06  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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	:	2.11
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)	:	2.11

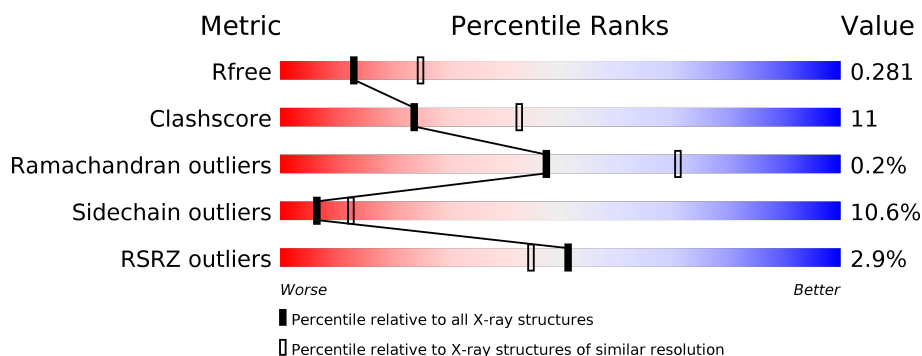
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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  $\leq 5\%$ . 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	461	<div> <div>3%</div> <div>69%</div> <div>25%</div> <div>• •</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3362 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 Protein DETOXIFICATION 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3362	2202	543	592	25			

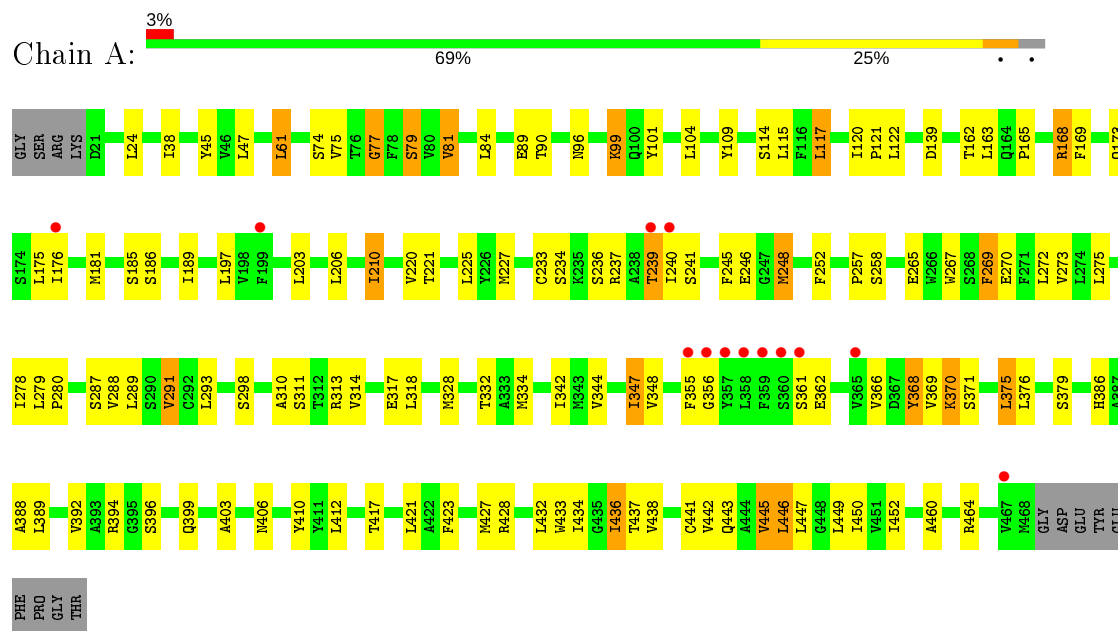
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	expression tag	UNP Q9C994
A	18	SER	-	expression tag	UNP Q9C994
A	19	ARG	-	expression tag	UNP Q9C994
A	36	ALA	PRO	engineered mutation	UNP Q9C994
A	474	PHE	-	expression tag	UNP Q9C994
A	475	PRO	-	expression tag	UNP Q9C994
A	476	GLY	-	expression tag	UNP Q9C994
A	477	THR	-	expression tag	UNP Q9C994

### 3 Residue-property plots [i](#)

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: Protein DETOXIFICATION 14



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.80 Å 86.78 Å 116.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 2.60 48.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.34-2.60) 98.5 (48.34-2.60)	Depositor EDS
$R_{merge}$	0.58	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.61 Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.224 , 0.276 0.227 , 0.281	Depositor DCC
$R_{free}$ test set	842 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3362	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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	0.45	0/3432	0.55	0/4657

There are no bond length outliers.

There are no bond angle outliers.

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	3362	0	3470	76	0
All	All	3362	0	3470	76	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 11.

All (76) 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:75:VAL:HG13	1:A:267:TRP:HD1	1.39	0.86
1:A:406:ASN:OD1	1:A:443:GLN:NE2	2.14	0.81
1:A:356:GLY:HA3	1:A:370:LYS:HE2	1.72	0.71
1:A:89:GLU:OE1	1:A:394:ARG:NH1	2.28	0.67
1:A:75:VAL:HG13	1:A:267:TRP:CD1	2.28	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:MET:O	1:A:332:THR:HG23	2.02	0.60
1:A:45:TYR:OH	1:A:298:SER:HB3	2.03	0.59
1:A:257:PRO:HB2	1:A:399:GLN:HB3	1.84	0.59
1:A:206:LEU:O	1:A:210:ILE:HG23	2.03	0.58
1:A:233:CYS:O	1:A:237:ARG:HB3	2.04	0.58
1:A:344:VAL:HA	1:A:347:ILE:HG22	1.85	0.58
1:A:258:SER:OG	1:A:399:GLN:HG2	2.05	0.57
1:A:101:TYR:O	1:A:236:SER:HA	2.06	0.56
1:A:75:VAL:HG21	1:A:270:GLU:HB2	1.88	0.55
1:A:245:PHE:HA	1:A:248:MET:HG3	1.87	0.55
1:A:368:TYR:O	1:A:371:SER:OG	2.17	0.54
1:A:366:VAL:O	1:A:370:LYS:HD2	2.08	0.54
1:A:278:ILE:HG13	1:A:423:PHE:HZ	1.72	0.54
1:A:433:TRP:O	1:A:437:THR:HG23	2.07	0.54
1:A:280:PRO:HB2	1:A:428:ARG:NH1	2.24	0.53
1:A:375:LEU:HD11	1:A:434:ILE:HG13	1.92	0.52
1:A:376:LEU:HB2	1:A:433:TRP:HH2	1.75	0.52
1:A:173:GLN:HB2	1:A:175:LEU:HG	1.92	0.52
1:A:280:PRO:HB2	1:A:428:ARG:HH12	1.75	0.51
1:A:433:TRP:O	1:A:436:ILE:HG22	2.11	0.50
1:A:74:SER:O	1:A:79:SER:HB2	2.12	0.50
1:A:442:VAL:HG12	1:A:446:LEU:HD22	1.94	0.49
1:A:120:ILE:HB	1:A:121:PRO:HD3	1.94	0.49
1:A:197:LEU:O	1:A:203:LEU:HB2	2.12	0.49
1:A:278:ILE:HG13	1:A:423:PHE:CZ	2.48	0.49
1:A:239:THR:HG23	1:A:241:SER:HB3	1.94	0.49
1:A:288:VAL:HG11	1:A:368:TYR:CE2	2.47	0.48
1:A:287:SER:O	1:A:291:VAL:HG12	2.14	0.48
1:A:162:THR:O	1:A:165:PRO:HD2	2.14	0.48
1:A:169:PHE:CE2	1:A:227:MET:HG3	2.48	0.48
1:A:293:LEU:HD12	1:A:293:LEU:O	2.15	0.46
1:A:318:LEU:HD12	1:A:396:SER:HA	1.96	0.46
1:A:114:SER:HB3	1:A:252:PHE:CE2	2.50	0.46
1:A:163:LEU:HB2	1:A:220:VAL:HG23	1.99	0.45
1:A:310:ALA:O	1:A:314:VAL:HG13	2.16	0.45
1:A:434:ILE:O	1:A:438:VAL:HG23	2.16	0.45
1:A:77:GLY:HA2	1:A:122:LEU:HD13	1.99	0.45
1:A:362:GLU:O	1:A:366:VAL:HG23	2.17	0.44
1:A:99:LYS:HD3	1:A:101:TYR:OH	2.18	0.44
1:A:356:GLY:CA	1:A:370:LYS:HE2	2.44	0.44
1:A:89:GLU:OE2	1:A:168:ARG:NH2	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:CYS:O	1:A:445:VAL:HG13	2.17	0.44
1:A:185:SER:OG	1:A:189:ILE:HD11	2.18	0.44
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.78	0.44
1:A:313:ARG:NH2	1:A:317:GLU:OE1	2.50	0.44
1:A:460:ALA:O	1:A:464:ARG:HG3	2.18	0.44
1:A:117:LEU:HA	1:A:117:LEU:HD12	1.80	0.44
1:A:288:VAL:HG23	1:A:369:VAL:HG23	1.99	0.43
1:A:421:LEU:HD22	1:A:427:MET:SD	2.58	0.43
1:A:96:ASN:HB2	1:A:104:LEU:HD11	2.01	0.43
1:A:221:THR:O	1:A:225:LEU:HG	2.19	0.43
1:A:344:VAL:HA	1:A:347:ILE:CG2	2.47	0.43
1:A:81:VAL:HG23	1:A:115:LEU:HD22	2.00	0.43
1:A:388:ALA:O	1:A:392:VAL:HG23	2.19	0.42
1:A:265:GLU:HB2	1:A:410:TYR:CZ	2.54	0.42
1:A:386:HIS:CG	1:A:443:GLN:HG2	2.55	0.42
1:A:61:LEU:O	1:A:61:LEU:HD22	2.19	0.42
1:A:270:GLU:O	1:A:273:VAL:HG22	2.20	0.42
1:A:318:LEU:CD1	1:A:396:SER:HA	2.50	0.41
1:A:348:VAL:HG12	1:A:355:PHE:CE2	2.56	0.41
1:A:248:MET:HB3	1:A:248:MET:HE3	1.75	0.41
1:A:447:LEU:HD23	1:A:447:LEU:HA	1.72	0.41
1:A:334:MET:HE1	1:A:389:LEU:HG	2.02	0.41
1:A:417:THR:HG21	1:A:438:VAL:HG21	2.03	0.41
1:A:109:TYR:CE2	1:A:240:ILE:HG12	2.56	0.41
1:A:288:VAL:O	1:A:291:VAL:HG13	2.21	0.41
1:A:272:LEU:HD22	1:A:432:LEU:HD22	2.03	0.40
1:A:452:ILE:HD13	1:A:452:ILE:HA	1.86	0.40
1:A:269:PHE:O	1:A:273:VAL:HG13	2.21	0.40
1:A:366:VAL:HG12	1:A:370:LYS:CD	2.52	0.40
1:A:403:ALA:O	1:A:406:ASN:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	446/461 (97%)	437 (98%)	8 (2%)	1 (0%)	47 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLY

### 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	358/372 (96%)	320 (89%)	38 (11%)	6 12

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	38	ILE
1	A	47	LEU
1	A	61	LEU
1	A	79	SER
1	A	81	VAL
1	A	84	LEU
1	A	90	THR
1	A	99	LYS
1	A	117	LEU
1	A	139	ASP
1	A	168	ARG
1	A	176	ILE
1	A	181	MET
1	A	186	SER
1	A	210	ILE
1	A	234	SER
1	A	239	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	246	GLU
1	A	248	MET
1	A	269	PHE
1	A	275	LEU
1	A	279	LEU
1	A	291	VAL
1	A	311	SER
1	A	342	ILE
1	A	347	ILE
1	A	361	SER
1	A	368	TYR
1	A	370	LYS
1	A	375	LEU
1	A	379	SER
1	A	412	LEU
1	A	436	ILE
1	A	445	VAL
1	A	446	LEU
1	A	449	LEU
1	A	450	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	448/461 (97%)	0.21	13 (2%) 51 45	29, 50, 76, 99	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	PHE	4.8
1	A	360	SER	3.8
1	A	239	THR	3.6
1	A	357	TYR	3.5
1	A	361	SER	3.5
1	A	240	ILE	3.1
1	A	467	VAL	2.7
1	A	358	LEU	2.6
1	A	355	PHE	2.5
1	A	365	VAL	2.2
1	A	199	PHE	2.2
1	A	356	GLY	2.1
1	A	176	ILE	2.1

### 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 ⓘ

There are no such residues in this entry.