



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3MKT / pdb_00003mkt
Title : Structure of a Cation-bound Multidrug and Toxin Compound Extrusion (MATE) transporter
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Deposited on : 2010-04-15
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

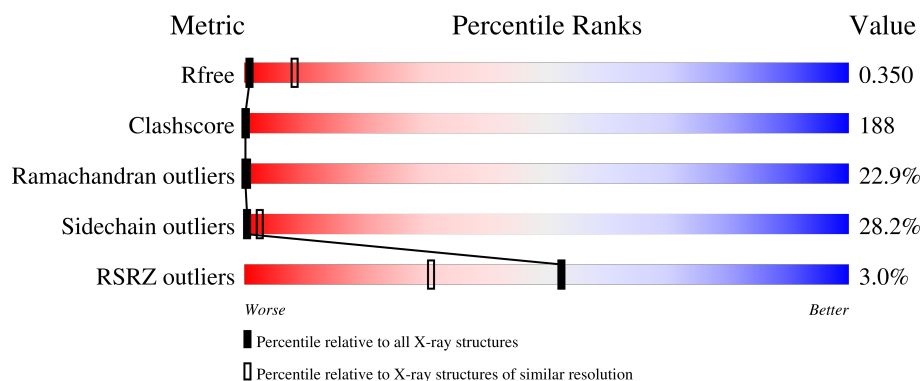
1 Overall quality at a glance

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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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 $\leq 5\%$. 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	460	
1	B	460	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 7011 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.

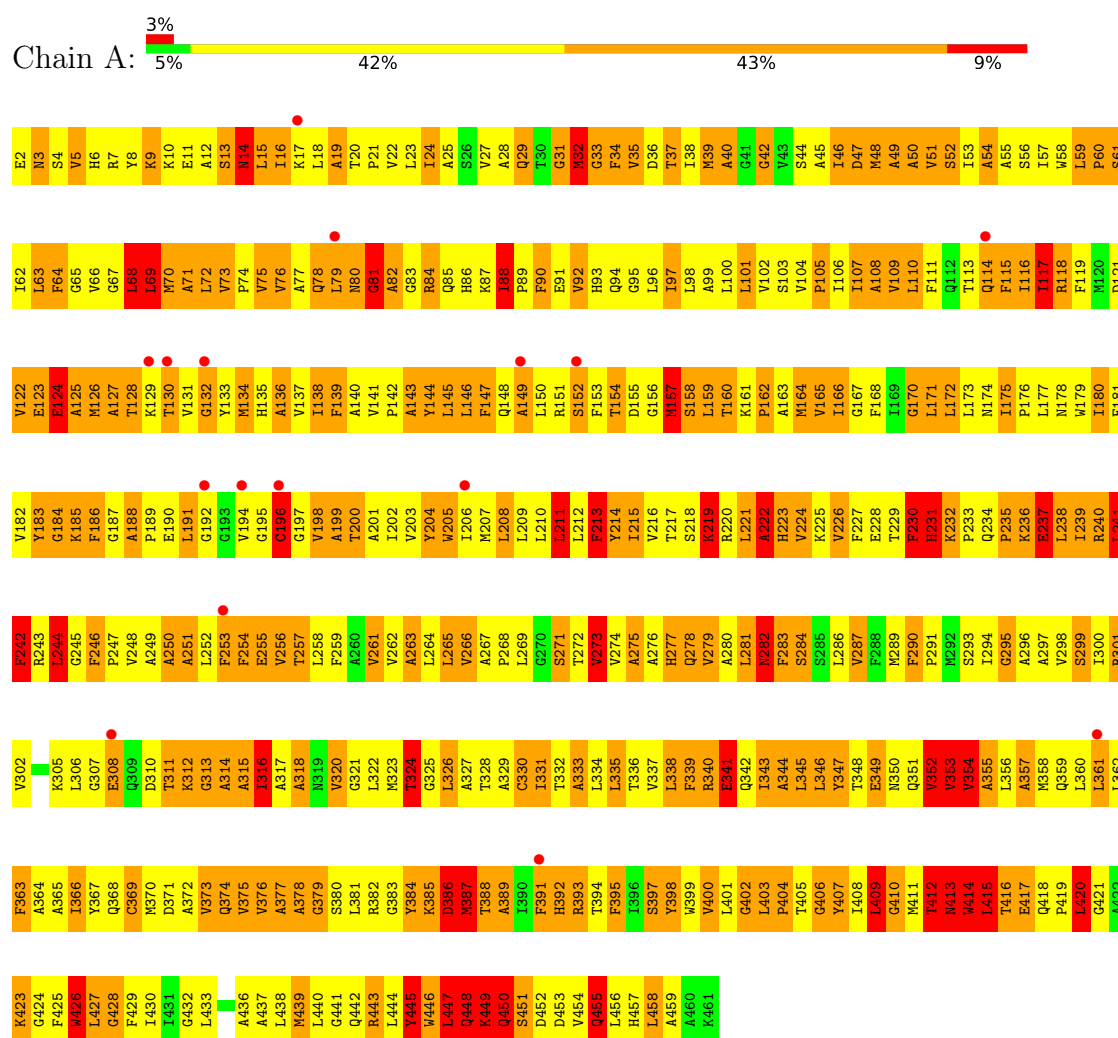
- Molecule 1 is a protein called Multi antimicrobial extrusion protein (Na(+)/drug antiporter) MATE-like MDR efflux pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3505	2326	569	589	21			
1	B	460	Total	C	N	O	S	0	0	0
			3506	2326	569	590	21			

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 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: Multi antimicrobial extrusion protein (Na(+))/drug antiporter) MATE-like MDR efflux pump



- Molecule 1: Multi antimicrobial extrusion protein (Na(+))/drug antiporter) MATE-like MDR efflux pump



G424	A364	R243	Y183	E123	I62	E2
F425	A365	L244	G184	E124	L63	N3
W426	I366	G245	K185	M126	F64	S4
L427	Y367	F246	F186	A127	G65	V5
G428	Q368	P247	K187	T128	V66	H6
F429	C369	V248	A188	T129	G67	R7
I430	M370	A249	P189	K129	L68	Y8
I431	D371	A250	E190	T130	L69	K9
G432	A372	A251	L191	V131	M70	K10
L433	V373	L252	G192	G132	A71	E11
	Q374	F253	G193	Y133	L72	A12
A436	V375	F254	V194	M134	V73	S13
A437	Y376	F255	G195	H135	P74	N14
L438	A377	V256	G186	A136	V75	L15
M439	A378	T257	I197	V137	V76	I16
L440	G379	L258	V198	I138	A77	K17
G441	S380	F259	A199	F139	Q78	L18
Q442	L381	A260	T200	A140	L79	A19
R443	R382	V261	A201	V141	N80	T20
L444	G383	V262	I202	P142	G81	P21
Y445	Y384	A263	V203	A143	A82	V22
W446	K385	L264	Y204	Y144	G83	L23
L447	D386	L265	W205	L145	R84	L24
Q448	M387	V266	I206	L146	Q85	A25
K449	T388	A267	M207	F147	H86	S26
Q450	A389	P268	L208	Q148	V27	V27
S451	I390	L269	L209	A149	A28	A28
D452	F391	G270	L210	L150	P89	Q29
D453	H392	S271	L211	R151	F90	T30
V454	R393	T272	L212	S152	E91	G31
Q455	T394	V273	F213	F153	V92	M32
L456	F395	V274	Y214	T154	H93	G33
H457	I396	A275	I215	D155	Q94	F34
L458	S397	A276	V216	G156	G95	V35
A459	Y398	H277	T217	M157	L96	D36
A460	W399	Q278	S218	S158	I97	T37
K461	V400	V279	K219	L159	I38	I38
	L401	A280	R220	T160	A99	M39
	G402	L281	L221	K161	L100	A40
	L403	V282	A222	P162	L101	G41
	P404	F283	H223	A163	V102	G42
	T405	S284	V224	M164	S103	V43
	G406	S285	K225	V165	V104	S44
	Y407	L286	V226	I166	P105	A45
	I408	V287	F227	G167	I106	T46
	L409	F288	E228	F168	I107	D47
	G410	M289	T229	I169	A108	M48
	M411	Q351	F290	G170	V109	A49
	T412	V352	H231	L171	L110	A50
M413	V353	W292	K232	L172	F111	V51
W414	V354	S293	P233	L173	Q112	S52
L415	A355	L294	Q234	N174	T113	I53
T416	L356	Q295	P235	I175	Q114	A54
E417	A357	A296	K236	P176	F115	A55
Q418	M358	A297	E237	L177	S56	S56
P419	Q359	V298	L238	T117	I57	I57
L420	L360	S299	I239	R118	W58	W58
G421	L361	I300	R240	F119	L59	L59
A422	L362	R301	L241	F181	P60	P60
K423	F363	V302	F242	V182	S61	S61

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.84Å 238.77Å 45.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 3.65 19.77 – 3.65	Depositor EDS
% Data completeness (in resolution range)	86.5 (19.77-3.65) 85.9 (19.77-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.312 , 0.343 0.312 , 0.350	Depositor DCC
R_{free} test set	794 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.861	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7011	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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	0.85	5/3585 (0.1%)	1.58	88/4879 (1.8%)
1	B	0.84	3/3586 (0.1%)	1.52	83/4879 (1.7%)
All	All	0.85	8/7171 (0.1%)	1.55	171/9758 (1.8%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	ILE	CA-CB	7.42	1.58	1.53
1	A	88	ILE	CA-CB	7.10	1.58	1.53
1	A	311	THR	CA-CB	5.55	1.61	1.53
1	B	222	ALA	CA-C	-5.52	1.45	1.52
1	A	138	ILE	CA-CB	5.38	1.61	1.54

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	N-CA-C	-21.58	92.17	113.10
1	B	75	VAL	N-CA-C	-19.77	93.92	112.90
1	B	136	ALA	N-CA-C	-16.19	93.04	111.82
1	A	223	HIS	N-CA-C	-15.82	88.94	111.56
1	A	136	ALA	N-CA-C	-15.59	93.73	111.82

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	3505	0	3677	1348	0
1	B	3506	0	3677	1350	0
All	All	7011	0	7354	2696	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 188.

The worst 5 of 2696 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:124:GLU:O	1:A:128:THR:HB	1.34	1.24
1:B:410:GLY:HA3	1:B:425:PHE:HB3	1.27	1.17
1:A:275:ALA:HA	1:A:353:VAL:HG11	1.30	1.14
1:A:410:GLY:HA3	1:A:425:PHE:HB3	1.26	1.13
1:B:165:VAL:HG13	1:B:166:ILE:N	1.61	1.13

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	458/460 (100%)	239 (52%)	111 (24%)	108 (24%)	0	0
1	B	458/460 (100%)	244 (53%)	112 (24%)	102 (22%)	0	0
All	All	916/920 (100%)	483 (53%)	223 (24%)	210 (23%)	0	0

5 of 210 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	15	LEU
1	A	35	VAL

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Mol	Chain	Res	Type
1	A	40	ALA
1	A	46	ILE

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	364/364 (100%)	262 (72%)	102 (28%)	0	2
1	B	364/364 (100%)	261 (72%)	103 (28%)	0	2
All	All	728/728 (100%)	523 (72%)	205 (28%)	0	2

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90	PHE
1	B	231	HIS
1	B	446	TRP
1	B	118	ARG
1	B	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	359	GLN
1	B	442	GLN
1	B	457	HIS
1	A	413	ASN
1	A	351	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 oligosaccharides 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	460/460 (100%)	0.19	16 (3%)	47 28	46, 126, 183, 286	0
1	B	460/460 (100%)	0.09	12 (2%)	57 34	56, 130, 193, 270	0
All	All	920/920 (100%)	0.14	28 (3%)	52 31	46, 129, 189, 286	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLN	4.6
1	A	130	THR	3.8
1	A	391	PHE	3.6
1	A	79	LEU	3.5
1	A	129	LYS	3.0

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 oligosaccharides 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.