



wwPDB X-ray Structure Validation Summary Report

May 12, 2020 – 11:24 pm BST

PDB ID : 3MKT
Title : Structure of a Cation-bound Multidrug and Toxin Compound Extrusion (MATE) transporter
Authors : He, X.; Szewczyk, P.; Karyakin, A.; Evin, M.; Hong, W.-X.; Zhang, Q.; Chang, G.
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 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

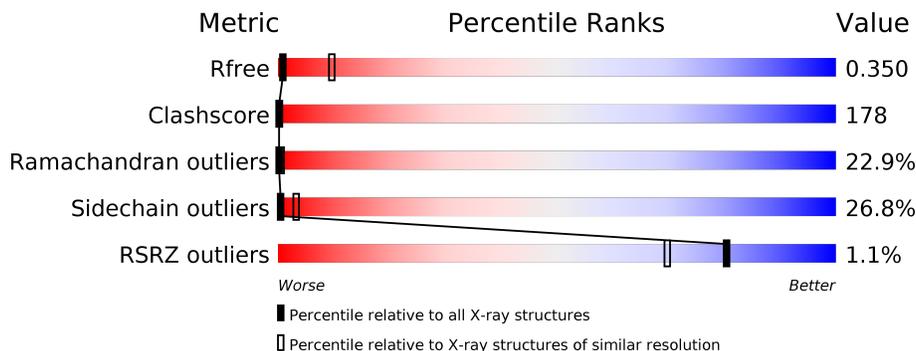
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)
RSRZ outliers	127900	1441 (3.82-3.50)

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 ≥ 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

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.

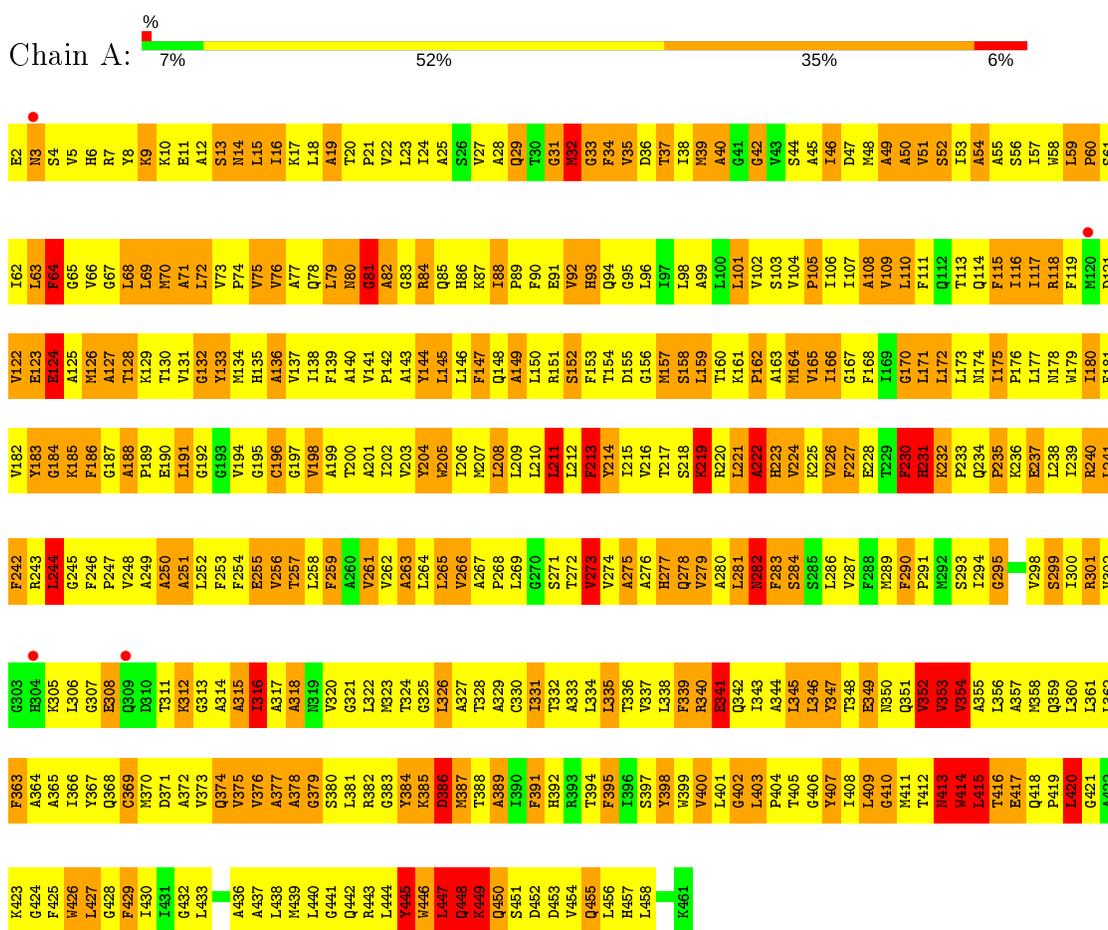
- Molecule 1 is a protein called Multi antimicrobial extrusion protein (Na(+)/drug antiporter) MATE-like MDR efflux pump.

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

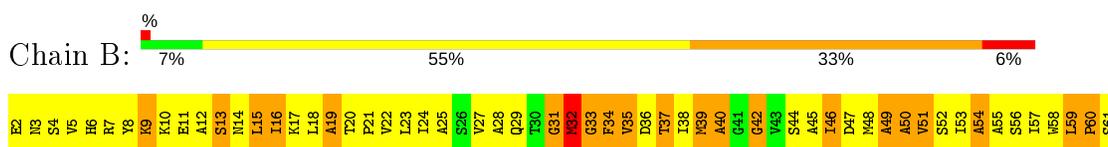
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



K423	F363	V302	F242	V182	V122	I62
G424	A364	K305	R243	Y183	E123	L63
F425	A365	L306	L244	K184	E124	F64
W426	I366	G307	G245	K185	A125	G65
L427	Y367	E308	F246	F186	M126	V66
G428	Q368	Q309	P247	F187	G127	G67
F429	C369	D310	V248	A188	T128	L68
I430	M370	D311	A249	P189	K129	L69
L431	D371	T311	A250	E190	L129	M70
G432	A372	K312	A251	L191	V131	A71
L433	V373	G313	L252	G192	G132	L72
A436	Q374	A314	F253	G193	Y133	V73
A437	A375	A315	F254	V194	M134	F74
L438	V376	R316	E255	G195	H135	V75
M439	A377	A317	V256	C196	A136	V76
L440	A378	A318	T257	C197	V137	A77
G441	G379	R319	L258	V198	I138	Q78
Q442	S380	V320	F259	A199	F139	L79
R443	L381	G321	V260	T200	A140	M80
L444	R382	L322	V261	A201	V141	G81
W445	G383	R323	V262	I202	P142	A82
W446	Y384	T324	A263	V203	A143	G83
L447	K385	G325	L264	Y204	Y144	R84
Q448	L386	L326	L265	V205	L145	Q85
K449	M387	A327	V266	V206	L146	H86
Q450	T388	T328	A267	V207	F147	K87
S451	A389	A329	P268	L208	Q148	I88
D452	I390	C330	L269	L209	A149	P89
D453	F391	L331	G270	L210	L150	F90
V454	R392	T332	S271	L211	R151	E91
Q455	R393	A333	T272	L212	S152	V92
L456	T394	L334	V273	F213	F153	H93
H457	F395	L335	V274	T214	T154	Q94
L458	I396	T336	A275	I215	D155	G95
A459	S397	V337	A276	V216	G156	L96
A460	Y398	L338	H277	T217	M157	I97
K461	Y399	F339	Q278	S218	S158	L98
	V400	R340	V279	R219	L159	A99
	L401	E341	A280	R220	T160	L100
	G402	Q342	L281	L221	K161	L101
	L403	L343	V282	A222	P162	V102
	P404	A344	F283	R223	A163	S103
	T405	L345	S284	V224	M164	V104
	G406	L346	S285	V225	V165	P105
	Y407	T347	L286	V226	L166	I106
	I408	T348	V287	V227	G167	I107
	L409	E349	F288	E228	F168	A108
	G410	M350	K289	T229	V169	V109
	M411	Q351	P290	F230	G170	L110
	T412	V352	P291	R231	L171	F111
	M413	V353	V292	K232	L172	Q112
	W414	S293	S293	P233	L173	T113
	L415	L294	L294	Q234	M174	Q114
	T416	L356	G295	P235	I175	F115
	E417	A357	A296	K236	P176	I116
	Q418	K358	A297	E237	L177	I117
	P419	Q359	V298	L238	M178	A118
	L420	L360	S299	L239	W179	F119
	G421	L361	T300	R240	I180	M120
	A422	L362	R301	L241	F181	D121

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 19.76 – 3.65	Depositor EDS
% Data completeness (in resolution range)	86.5 (19.77-3.65) 86.6 (19.76-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.61Å)	Xtrriage
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	Xtrriage
Anisotropy	0.861	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 85.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹ Intensities estimated from amplitudes.

² 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	0.66	1/3585 (0.0%)	1.01	20/4879 (0.4%)
1	B	0.65	0/3586	0.94	13/4879 (0.3%)
All	All	0.65	1/7171 (0.0%)	0.98	33/9758 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	TRP	CB-CG	5.24	1.59	1.50

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	TRP	CB-CA-C	-10.02	90.37	110.40
1	A	449	LYS	N-CA-CB	-9.07	94.27	110.60
1	A	352	VAL	CB-CA-C	8.71	127.94	111.40
1	A	353	VAL	N-CA-CB	-8.27	93.31	111.50
1	A	223	HIS	N-CA-C	-8.17	88.94	111.00

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	1279	0
1	B	3506	0	3677	1285	0
All	All	7011	0	7354	2562	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 178.

The worst 5 of 2562 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:A:165:VAL:HG13	1:A:166:ILE:N	1.63	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	1
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
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%)	267 (73%)	97 (27%)	0	3
1	B	364/364 (100%)	266 (73%)	98 (27%)	0	3
All	All	728/728 (100%)	533 (73%)	195 (27%)	0	3

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	420	LEU
1	B	90	PHE
1	B	409	LEU
1	A	427	LEU
1	B	32	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	B	14	ASN
1	B	450	GLN
1	A	457	HIS
1	B	78	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, 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%)	-0.56	4 (0%) 84 74	46, 126, 183, 286	0
1	B	460/460 (100%)	-0.58	6 (1%) 77 65	56, 130, 193, 270	0
All	All	920/920 (100%)	-0.57	10 (1%) 80 70	46, 129, 189, 286	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	MET	5.2
1	B	419	PRO	4.9
1	A	120	MET	3.6
1	B	309	GLN	2.4
1	A	304	HIS	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.