



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3MKU
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 : 4.20 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
<http://wwpdb.org/validation/2016/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
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

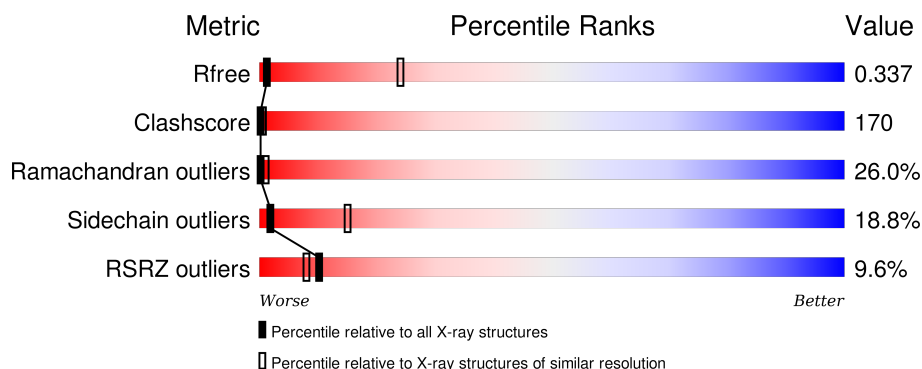
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	460	<div> <div>12%</div> <div>5% 58% 33% .</div> </div>
1	B	460	<div> <div>7%</div> <div>. 59% 33% .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7013 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			

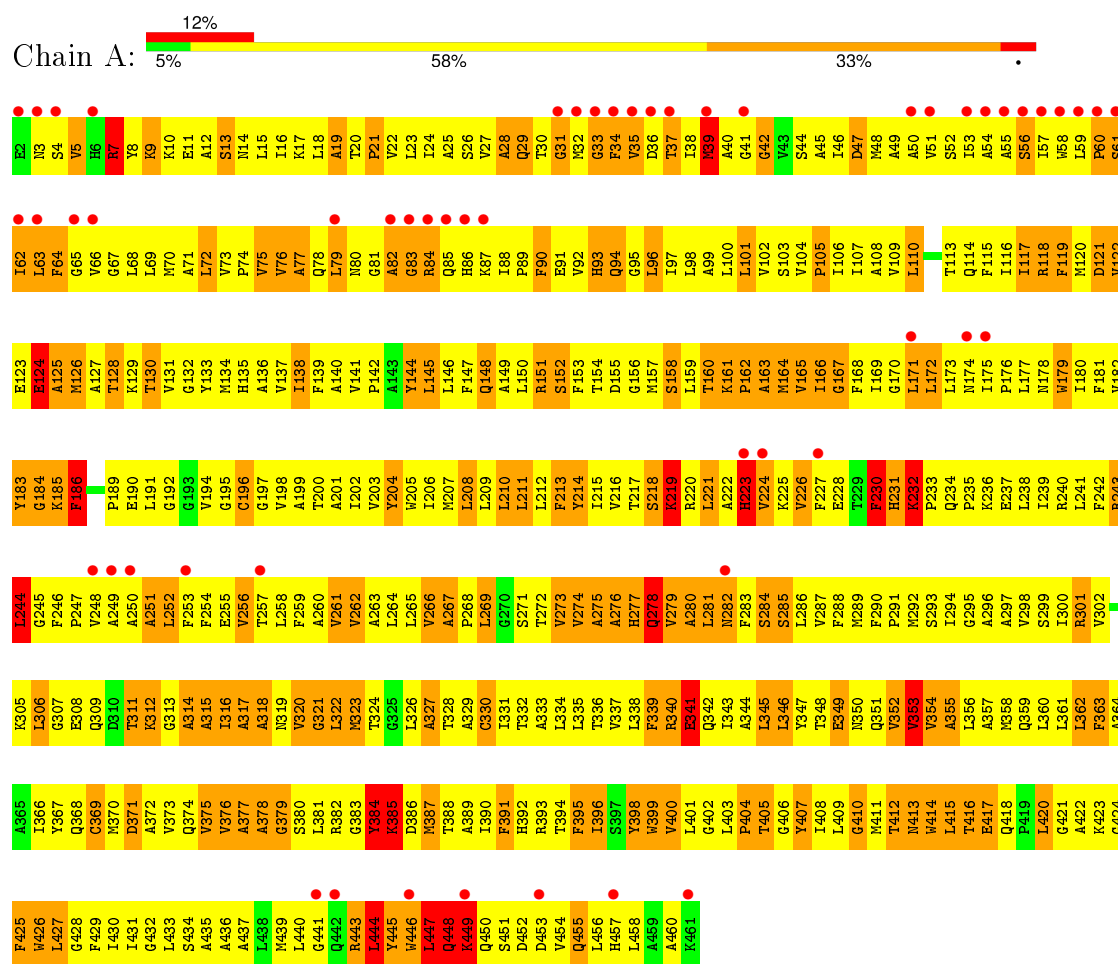
- Molecule 2 is RUBIDIUM ION (three-letter code: Rb) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Rb	0	0
			1	1		
2	A	1	Total	Rb	0	0
			1	1		

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



G424	F425	W426	L427	G428	F429	I430	I431	G432	L433	S434	A435	A436	A437	L438	M439	L440	G441	G442	R443	L444	Y445	W446	L447	Q448	K449	Q450	S451	D452	D453	V454	Q455	L456	H457	L458	A459	A460	K461																									
A364	A365	I366	Y367	Q368	C369	M370	D371	A372	V373	S374	V375	V376	A377	A378	G379	S380	L381	R382	G383	Y384	R385	D386	M387	T388	A389	I390	F391	R392	R393	T394	F395	I396	S397	Y398	W399	V400	L401	G402	L403	P404	T405	G406	Y407	I408	L409	G410	M411	T412	M413	W414	L415	T416	E417	Q418	R419	L420	G421	A422	K423			
V302	R305	L306	G307	E308	Q309	D310	T311	G312	G313	A314	A315	T316	A317	A318	N319	G320	G321	A260	V261	V262	A263	L264	L265	V266	A267	P268	L269	G270	S271	T272	V273	V274	A275	A276	H277	Q278	V279	A280	L281	N282	F283	S284	S285	L286	V287	F288	N289	F290	P291	M292	S293	L294	G295	A296	A297	V298	S299	I300	R301			
F242	R243	L244	G245	F246	P247	V248	A249	A250	A251	L252	F253	F254	E255	V256	T257	L258	F259	A260	V261	V262	A263	L264	L265	V266	A267	P268	L269	G270	S271	T272	V273	V274	A275	A276	H277	Q278	V279	A280	L281	N282	F283	S284	S285	L286	V287	F288	N289	F290	P291	M292	S293	L294	G295	A296	A297	V298	S299	I300	R301			
V182	Y183	G184	K185	F186	G187	A188	P189	E190	L191	G192	G193	V194	G195	C196	G197	V198	I199	T200	A201	I202	V203	A143	Y204	W205	L206	M207	L208	L209	L210	L211	L212	F213	Y214	I215	D216	G217	M217	S218	R219	R220	L221	A222	A163	M164	V224	K225	V226	F227	E228	T229	F230	H231	K232	P233	Q234	P235	K236	E237	L238	I239	R240	L241
I62	L63	F64	G65	V66	G67	L68	L69	M70	A71	L72	V73	P74	V75	V76	A77	Q78	L79	N80	G81	A82	G83	R84	Q85	H86	K87	P88	P89	F90	E91	V92	H93	Q94	L96	G95	I97	L98	A99	L100	L101	V102	S103	V104	P105	I106	I107	A108	V109	L110	F111	Q112	T113	Q114	F115	I116	I117	R118	F119	M120	D121			
V122	E123	E124	A125	M126	A127	T128	K129	T130	V131	G132	Y133	M134	H135	A136	V137	I138	F139	A140	V141	F142	Y144	L145	L146	F147	Q148	A149	L150	R151	S152	F153	T154	D155	G156	M157	S158	L159	T160	K161	P162	A163	M164	V165	I166	F168	I169	G170	L171	L172	L173	M174	F175	P176	L177	M178	W179	I180	F181					

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.80Å 241.85Å 46.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.20 133.33 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-4.20) 99.0 (133.33-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 4.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.309 , 0.342 0.310 , 0.337	Depositor DCC
R_{free} test set	683 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	105.5	Xtriage
Anisotropy	1.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 145.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	1 of 15850 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RB

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	0.65	0/3585	0.97	13/4879 (0.3%)
1	B	0.64	0/3586	0.93	9/4879 (0.2%)
All	All	0.64	0/7171	0.95	22/9758 (0.2%)

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	B	0	2

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	353	VAL	CB-CA-C	-8.84	94.61	111.40
1	A	410	GLY	N-CA-C	-8.24	92.50	113.10
1	A	384	TYR	CB-CA-C	7.94	126.28	110.40
1	B	410	GLY	N-CA-C	-7.78	93.65	113.10
1	A	447	LEU	N-CA-C	-7.57	90.56	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	TYR	Sidechain
1	B	144	TYR	Sidechain

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	3676	1224	0
1	B	3506	0	3676	1223	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	7013	0	7352	2440	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 170.

The worst 5 of 2440 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:447:LEU:CD1	1:A:450:GLN:HE21	1.27	1.48
1:A:447:LEU:CD1	1:A:450:GLN:NE2	1.96	1.27
1:A:447:LEU:HD13	1:A:450:GLN:NE2	1.50	1.24
1:B:162:PRO:O	1:B:165:VAL:HG12	1.38	1.17
1:A:320:VAL:HG13	1:A:321:GLY:H	1.04	1.17

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%)	218 (48%)	118 (26%)	122 (27%)	0 1
1	B	458/460 (100%)	221 (48%)	121 (26%)	116 (25%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	916/920 (100%)	439 (48%)	239 (26%)	238 (26%)	0 1

5 of 238 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	35	VAL
1	A	56	SER
1	A	76	VAL
1	A	121	ASP

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	364/364 (100%)	296 (81%)	68 (19%)	2 15
1	B	364/364 (100%)	295 (81%)	69 (19%)	2 14
All	All	728/728 (100%)	591 (81%)	137 (19%)	2 15

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	425	PHE
1	B	63	LEU
1	B	407	TYR
1	A	427	LEU
1	B	14	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	B	14	ASN
1	B	455	GLN

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Mol	Chain	Res	Type
1	A	455	GLN
1	A	457	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.18	54 (11%) 6 6	34, 111, 174, 267	0
1	B	460/460 (100%)	0.02	34 (7%) 17 13	28, 117, 180, 253	0
All	All	920/920 (100%)	0.10	88 (9%) 10 8	28, 114, 180, 267	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	GLN	7.9
1	A	36	ASP	7.0
1	B	83	GLY	6.1
1	A	84	ARG	5.5
1	B	82	ALA	5.4

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	RB	B	5002	1/1	0.66	0.20	-	186,186,186,186	0
2	RB	A	5001	1/1	0.80	0.11	-	182,182,182,182	0

6.5 Other polymers [i](#)

There are no such residues in this entry.