



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 08:02 PM UTC

PDB ID : 3MKU / pdb_00003mku
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

<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

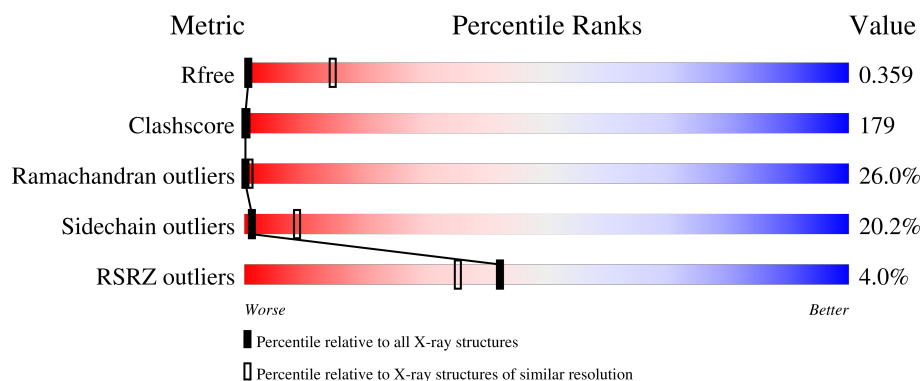
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	4% 46% 43% 7%
1	B	460	4% 49% 41% 7%

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			

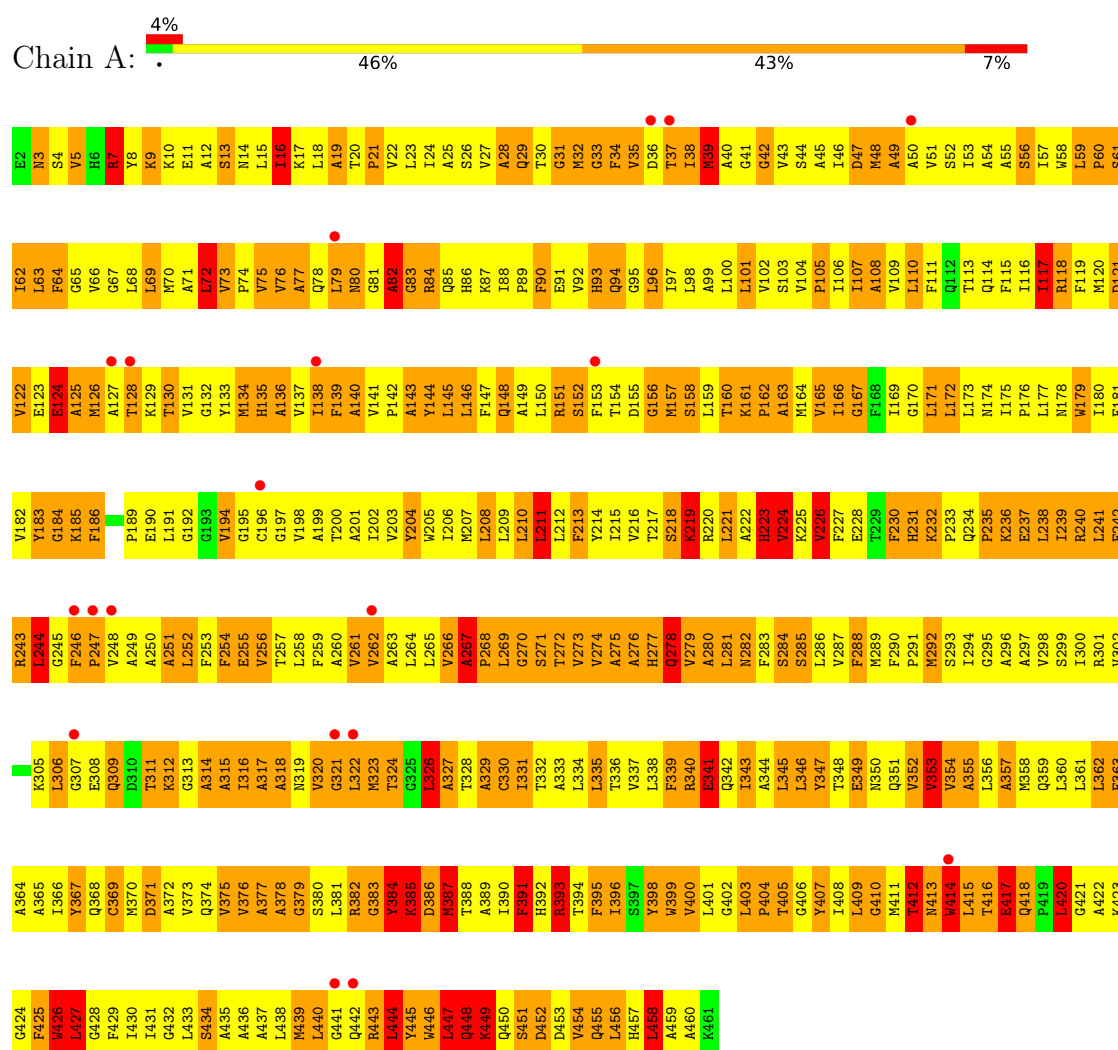
- Molecule 2 is RUBIDIUM ION (CCD ID: RB) (formula: Rb).

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

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



K423	F363	V302	F242	V182	V122	I62	E2
G424	A364	K305	R243	Y183	E123	L63	N3
F425	A365	K306	L244	G184	E124	F64	S4
W426	I366	L306	G245	K185	M126	G65	V5
L427	Y367	G307	F246	F186	A127	V66	H6
G428	Q368	E308	P247	G187	T128	G67	R7
F429	C369	Q309	V248	A188	K129	L68	Y8
I430	M370	D310	A249	P189	L130	L69	K9
I431	D371	T311	A250	E190	T130	M70	K10
G432	A372	K312	A251	L191	V131	A71	E11
L433	V373	G313	L252	G192	G132	L72	A12
S434	Q374	A314	F253	G193	V133	V73	S13
A435	V375	A315	F254	V194	M134	P74	N14
A436	V376	I316	E255	G195	H135	V75	L15
A437	A377	A317	V256	C196	A136	V76	I16
L438	A378	A318	T257	G197	V137	A77	K17
M439	G379	N319	L258	V198	I138	Q78	L18
L440	S380	V320	F259	A199	F139	L79	A19
G441	L381	G321	A260	T200	A140	N80	T20
Q442	R382	L322	V261	A201	V141	G81	P21
R443	G383	M323	V262	I202	P142	A82	V22
L444	Y384	T324	A263	V203	A143	G83	L23
Y445	K385	G325	L264	Y204	Y144	R84	I24
W446	D386	L326	L265	W205	L145	Q85	A25
L447	K387	A327	V266	L206	L146	H86	S26
Q448	T388	T328	A267	W207	F147	K87	V27
R449	A389	A329	P268	L208	Q148	I88	A28
Q450	I390	C330	L269	L209	A149	P89	Q29
S451	F391	I331	G270	L210	L150	F90	T30
D452	H392	T332	S271	L211	R151	E91	G31
D453	R393	A333	T272	L212	S152	V92	M32
W454	T394	L334	V273	F213	F153	H93	G33
Q455	F395	L335	V274	T214	T154	Q94	F34
L456	I396	V337	A275	I215	D155	G95	V35
H457	S397	V337	A276	V216	G156	L96	D36
L458	Y398	L338	H277	T217	M157	I97	T37
A459	W399	F339	Q278	S218	S158	L98	I38
A460	V400	R340	V279	K219	A99	A99	K39
K461	L401	E341	A280	R220	L100	A40	A40
	G402	Q342	L281	L221	K161	L101	G41
	L403	I343	N282	A222	P162	V102	G42
	P404	A344	F283	R223	A163	S103	V43
	T405	L345	S284	V224	M164	V104	S44
	G406	L346	S285	K225	V165	P105	A45
	Y407	Y347	L286	V226	I166	I106	I46
	I408	T348	V287	F227	G167	I107	D47
	L409	E349	F288	E228	F168	A108	M48
	G410	N350	M289	T229	I169	V109	A49
	M411	Q351	F290	F230	G170	L110	A50
	T412	V352	P291	H231	L171	F111	V51
	N413	V353	M292	K232	L172	Q112	S52
	W414	S354	S293	F233	L173	T113	I53
	L415	A355	I294	Q234	N174	Q114	A54
	T416	L356	G295	P235	I175	F115	A55
	E417	A357	A296	K236	P176	I116	S56
	Q418	M358	A297	E237	L177	I117	I57
	F419	Q359	V298	L238	N178	R118	W58
	L420	L360	S299	I239	W179	F119	L59
	G421	L361	I300	R240	I180	M120	P60
	A422	L362	R301	L241	F181	D121	S61

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 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 20.00 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-4.20) 97.8 (20.00-4.20)	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	Depositor
R, R_{free}	0.309 , 0.342 0.324 , 0.359	Depositor DCC
R_{free} test set	791 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	105.5	Xtriage
Anisotropy	1.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.08 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.84	3/3585 (0.1%)	1.49	89/4879 (1.8%)
1	B	0.83	4/3586 (0.1%)	1.46	75/4879 (1.5%)
All	All	0.83	7/7171 (0.1%)	1.47	164/9758 (1.7%)

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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	VAL	CA-CB	7.47	1.57	1.54
1	A	157	MET	SD-CE	7.06	1.97	1.79
1	B	294	ILE	CA-CB	6.63	1.61	1.54
1	A	32	MET	SD-CE	5.62	1.93	1.79
1	B	138	ILE	CA-CB	5.41	1.61	1.54

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ASN	N-CA-C	-14.85	95.10	111.14
1	B	413	ASN	N-CA-C	-14.25	95.75	111.14
1	A	236	LYS	N-CA-C	-12.78	97.81	113.41
1	B	236	LYS	N-CA-C	-12.50	98.16	113.41
1	A	75	VAL	N-CA-C	-12.17	95.03	113.16

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

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	1286	0
1	B	3506	0	3676	1292	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	7013	0	7352	2571	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 179.

The worst 5 of 2571 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:A:447:LEU:C	1:A:447:LEU:HD12	1.65	1.19
1:B:162:PRO:O	1:B:165:VAL:HG12	1.38	1.17

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	458/460 (100%)	218 (48%)	118 (26%)	122 (27%)	0	0
1	B	458/460 (100%)	221 (48%)	121 (26%)	116 (25%)	0	1
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 [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%)	292 (80%)	72 (20%)	1	9
1	B	364/364 (100%)	289 (79%)	75 (21%)	1	7
All	All	728/728 (100%)	581 (80%)	147 (20%)	1	9

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	312	LYS
1	B	449	LYS
1	B	341	GLU
1	B	398	TYR
1	A	385	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	14	ASN
1	B	114	GLN
1	B	359	GLN
1	B	85	GLN
1	B	148	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](#)

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 [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%)	0.28	19 (4%) 41 35	34, 111, 174, 267	0
1	B	460/460 (100%)	0.28	18 (3%) 43 36	28, 117, 180, 253	0
All	All	920/920 (100%)	0.28	37 (4%) 42 35	28, 114, 180, 267	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	THR	5.6
1	B	244	LEU	4.7
1	B	325	GLY	4.6
1	A	196	CYS	4.5
1	B	379	GLY	4.3

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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	RB	A	5001	1/1	0.82	0.17	182,182,182,182	0
2	RB	B	5002	1/1	0.82	0.25	186,186,186,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.