



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:53 PM UTC

PDB ID : 1VF7 / pdb_00001vf7
Title : Crystal structure of the membrane fusion protein, MexA of the multidrug transporter
Authors : Akama, H.; Matsuura, T.; Kashiwagi, S.; Yoneyama, H.; Tsukihara, T.; Nakagawa, A.; Nakae, T.
Deposited on : 2004-04-09
Resolution : 2.40 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

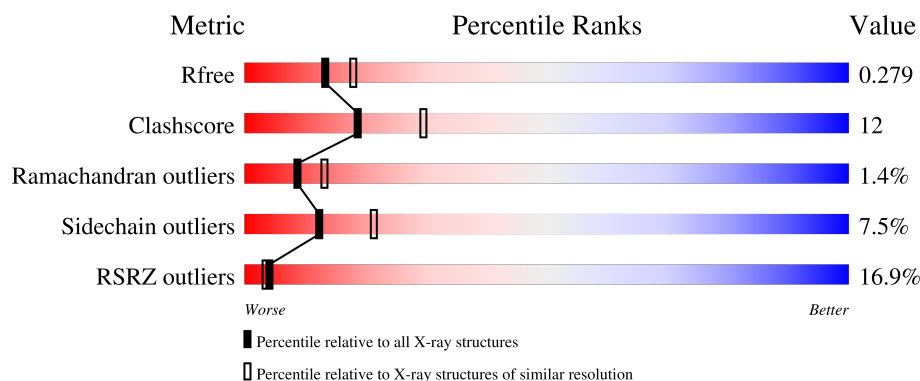
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	369	17% 43% 18% • 36%
1	B	369	6% 48% 12% • • 36%
1	C	369	7% 48% 15% • • 33%
1	D	369	4% 44% 16% • • 36%
1	E	369	8% 45% 18% • • 32%

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Mol	Chain	Length	Quality of chain
1	F	369	
1	G	369	
1	H	369	
1	I	369	
1	J	369	
1	K	369	
1	L	369	
1	M	369	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23655 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 Multidrug resistance protein mexA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1816	1127	327	360	2			
1	B	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	C	246	Total	C	N	O	S	0	0	0
			1885	1173	339	371	2			
1	D	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	E	252	Total	C	N	O	S	0	0	0
			1928	1198	348	380	2			
1	F	233	Total	C	N	O	S	0	0	0
			1788	1110	323	353	2			
1	G	237	Total	C	N	O	S	0	0	0
			1819	1130	327	360	2			
1	H	241	Total	C	N	O	S	0	0	0
			1846	1146	332	366	2			
1	I	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	J	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	K	232	Total	C	N	O	S	0	0	0
			1779	1105	321	351	2			
1	L	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	M	232	Total	C	N	O	S	0	0	0
			1779	1105	321	351	2			

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	cloning artifact	UNP P52477
A	-1	GLU	-	cloning artifact	UNP P52477
A	0	SER	-	cloning artifact	UNP P52477

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP P52477
A	361	HIS	-	expression tag	UNP P52477
A	362	HIS	-	expression tag	UNP P52477
A	363	HIS	-	expression tag	UNP P52477
A	364	HIS	-	expression tag	UNP P52477
A	365	HIS	-	expression tag	UNP P52477
A	366	HIS	-	expression tag	UNP P52477
B	-2	ALA	-	cloning artifact	UNP P52477
B	-1	GLU	-	cloning artifact	UNP P52477
B	0	SER	-	cloning artifact	UNP P52477
B	1	SER	-	cloning artifact	UNP P52477
B	361	HIS	-	expression tag	UNP P52477
B	362	HIS	-	expression tag	UNP P52477
B	363	HIS	-	expression tag	UNP P52477
B	364	HIS	-	expression tag	UNP P52477
B	365	HIS	-	expression tag	UNP P52477
B	366	HIS	-	expression tag	UNP P52477
C	-2	ALA	-	cloning artifact	UNP P52477
C	-1	GLU	-	cloning artifact	UNP P52477
C	0	SER	-	cloning artifact	UNP P52477
C	1	SER	-	cloning artifact	UNP P52477
C	361	HIS	-	expression tag	UNP P52477
C	362	HIS	-	expression tag	UNP P52477
C	363	HIS	-	expression tag	UNP P52477
C	364	HIS	-	expression tag	UNP P52477
C	365	HIS	-	expression tag	UNP P52477
C	366	HIS	-	expression tag	UNP P52477
D	-2	ALA	-	cloning artifact	UNP P52477
D	-1	GLU	-	cloning artifact	UNP P52477
D	0	SER	-	cloning artifact	UNP P52477
D	1	SER	-	cloning artifact	UNP P52477
D	361	HIS	-	expression tag	UNP P52477
D	362	HIS	-	expression tag	UNP P52477
D	363	HIS	-	expression tag	UNP P52477
D	364	HIS	-	expression tag	UNP P52477
D	365	HIS	-	expression tag	UNP P52477
D	366	HIS	-	expression tag	UNP P52477
E	-2	ALA	-	cloning artifact	UNP P52477
E	-1	GLU	-	cloning artifact	UNP P52477
E	0	SER	-	cloning artifact	UNP P52477
E	1	SER	-	cloning artifact	UNP P52477
E	361	HIS	-	expression tag	UNP P52477

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Chain	Residue	Modelled	Actual	Comment	Reference
E	362	HIS	-	expression tag	UNP P52477
E	363	HIS	-	expression tag	UNP P52477
E	364	HIS	-	expression tag	UNP P52477
E	365	HIS	-	expression tag	UNP P52477
E	366	HIS	-	expression tag	UNP P52477
F	-2	ALA	-	cloning artifact	UNP P52477
F	-1	GLU	-	cloning artifact	UNP P52477
F	0	SER	-	cloning artifact	UNP P52477
F	1	SER	-	cloning artifact	UNP P52477
F	361	HIS	-	expression tag	UNP P52477
F	362	HIS	-	expression tag	UNP P52477
F	363	HIS	-	expression tag	UNP P52477
F	364	HIS	-	expression tag	UNP P52477
F	365	HIS	-	expression tag	UNP P52477
F	366	HIS	-	expression tag	UNP P52477
G	-2	ALA	-	cloning artifact	UNP P52477
G	-1	GLU	-	cloning artifact	UNP P52477
G	0	SER	-	cloning artifact	UNP P52477
G	1	SER	-	cloning artifact	UNP P52477
G	361	HIS	-	expression tag	UNP P52477
G	362	HIS	-	expression tag	UNP P52477
G	363	HIS	-	expression tag	UNP P52477
G	364	HIS	-	expression tag	UNP P52477
G	365	HIS	-	expression tag	UNP P52477
G	366	HIS	-	expression tag	UNP P52477
H	-2	ALA	-	cloning artifact	UNP P52477
H	-1	GLU	-	cloning artifact	UNP P52477
H	0	SER	-	cloning artifact	UNP P52477
H	1	SER	-	cloning artifact	UNP P52477
H	361	HIS	-	expression tag	UNP P52477
H	362	HIS	-	expression tag	UNP P52477
H	363	HIS	-	expression tag	UNP P52477
H	364	HIS	-	expression tag	UNP P52477
H	365	HIS	-	expression tag	UNP P52477
H	366	HIS	-	expression tag	UNP P52477
I	-2	ALA	-	cloning artifact	UNP P52477
I	-1	GLU	-	cloning artifact	UNP P52477
I	0	SER	-	cloning artifact	UNP P52477
I	1	SER	-	cloning artifact	UNP P52477
I	361	HIS	-	expression tag	UNP P52477
I	362	HIS	-	expression tag	UNP P52477
I	363	HIS	-	expression tag	UNP P52477

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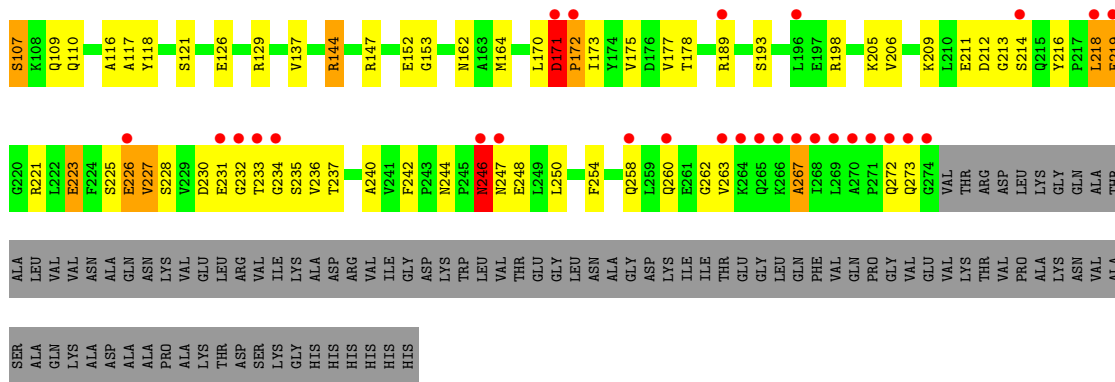
Chain	Residue	Modelled	Actual	Comment	Reference
I	364	HIS	-	expression tag	UNP P52477
I	365	HIS	-	expression tag	UNP P52477
I	366	HIS	-	expression tag	UNP P52477
J	-2	ALA	-	cloning artifact	UNP P52477
J	-1	GLU	-	cloning artifact	UNP P52477
J	0	SER	-	cloning artifact	UNP P52477
J	1	SER	-	cloning artifact	UNP P52477
J	361	HIS	-	expression tag	UNP P52477
J	362	HIS	-	expression tag	UNP P52477
J	363	HIS	-	expression tag	UNP P52477
J	364	HIS	-	expression tag	UNP P52477
J	365	HIS	-	expression tag	UNP P52477
J	366	HIS	-	expression tag	UNP P52477
K	-2	ALA	-	cloning artifact	UNP P52477
K	-1	GLU	-	cloning artifact	UNP P52477
K	0	SER	-	cloning artifact	UNP P52477
K	1	SER	-	cloning artifact	UNP P52477
K	361	HIS	-	expression tag	UNP P52477
K	362	HIS	-	expression tag	UNP P52477
K	363	HIS	-	expression tag	UNP P52477
K	364	HIS	-	expression tag	UNP P52477
K	365	HIS	-	expression tag	UNP P52477
K	366	HIS	-	expression tag	UNP P52477
L	-2	ALA	-	cloning artifact	UNP P52477
L	-1	GLU	-	cloning artifact	UNP P52477
L	0	SER	-	cloning artifact	UNP P52477
L	1	SER	-	cloning artifact	UNP P52477
L	361	HIS	-	expression tag	UNP P52477
L	362	HIS	-	expression tag	UNP P52477
L	363	HIS	-	expression tag	UNP P52477
L	364	HIS	-	expression tag	UNP P52477
L	365	HIS	-	expression tag	UNP P52477
L	366	HIS	-	expression tag	UNP P52477
M	-2	ALA	-	cloning artifact	UNP P52477
M	-1	GLU	-	cloning artifact	UNP P52477
M	0	SER	-	cloning artifact	UNP P52477
M	1	SER	-	cloning artifact	UNP P52477
M	361	HIS	-	expression tag	UNP P52477
M	362	HIS	-	expression tag	UNP P52477
M	363	HIS	-	expression tag	UNP P52477
M	364	HIS	-	expression tag	UNP P52477
M	365	HIS	-	expression tag	UNP P52477

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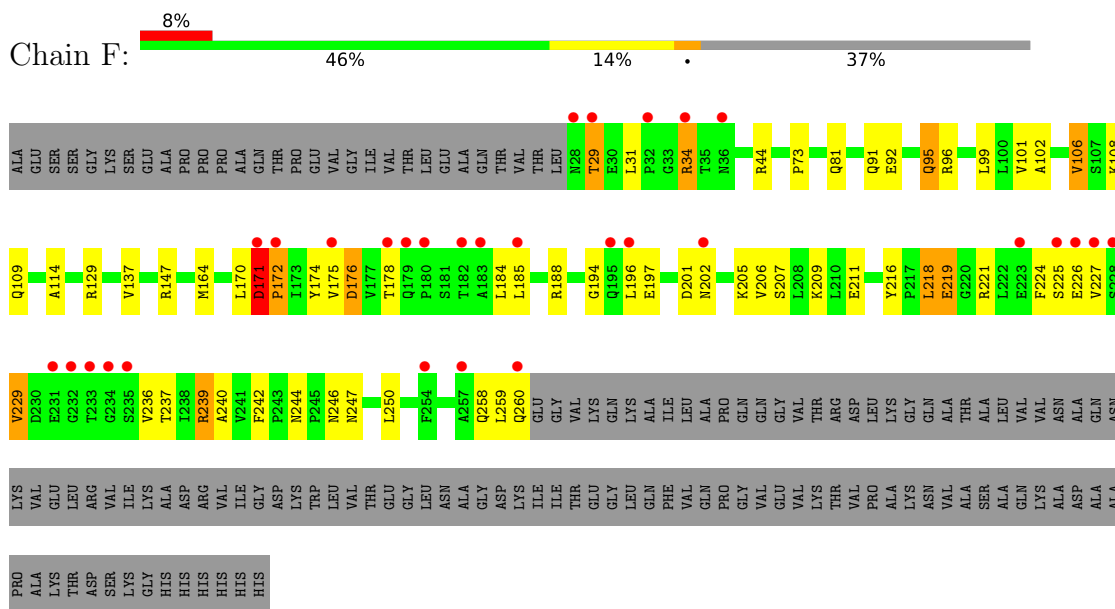
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Chain	Residue	Modelled	Actual	Comment	Reference
M	366	HIS	-	expression tag	UNP P52477

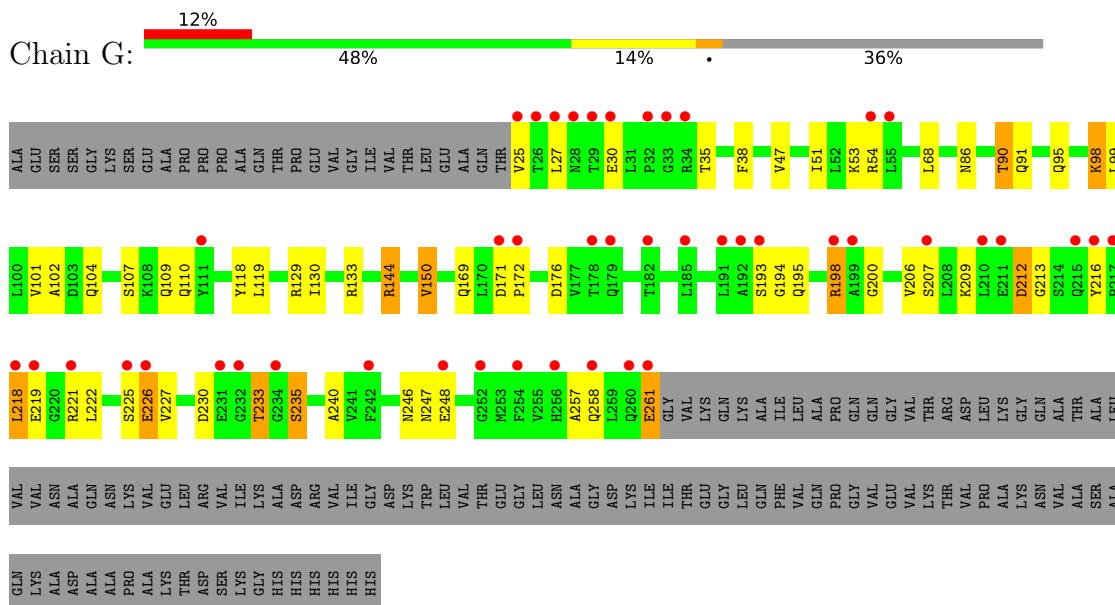
Chain E: 



- Molecule 1: Multidrug resistance protein mexA



- Molecule 1: Multidrug resistance protein mexA



[illegible]

Chain I:

6% 47% 13% 36%

ALA GLU SER SER GLY LYS SER GLU ALA PRO PRO PRO PRO ALA ALA GLN THR PRO PRO GLU VAL GLY ILE VAL THR LEU GLU ALA GLN THR VAL T26 T27 T28 T29 T30 T31 T32 T33 T34 T35 T36 T37 T38 T39 T40 T41 T42 T43 T44 T45 T46 T47 T48 T49 T50 T51 T52 T53 T54 T55 T56 T57 T58 T59 T60 T61 T62 T63 T64 T65 T66 T67 T68 T69 T70 T71 T72 T73 T74 T75 T76 T77 T78 T79 T80 T81 T82 T83 T84 T85 T86 T87 T88 T89 T90 T91 T92 T93 T94 T95 T96 T97 T98 T99 T100

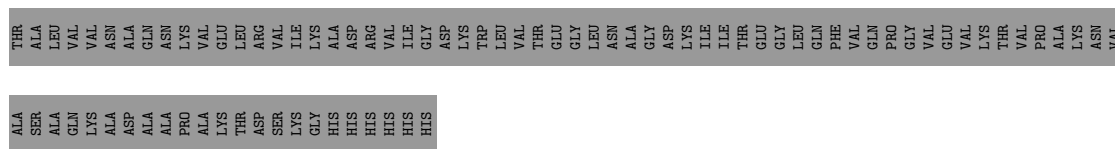
Chain J:

14% 49% 13% 36%

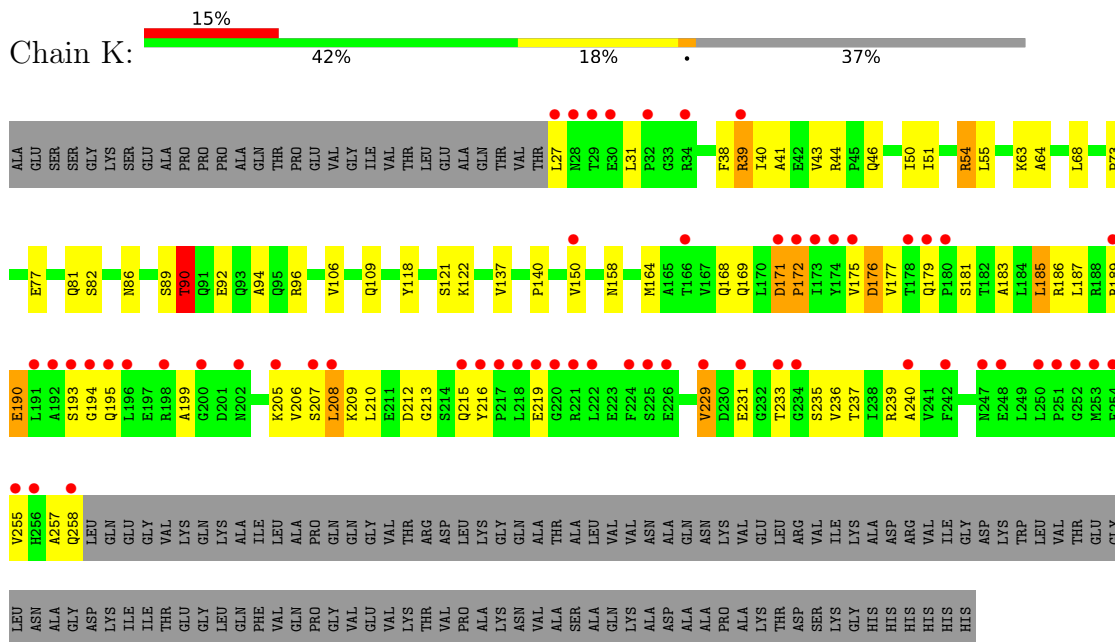
ALA
GLU
SER
SER
GLY
GLY
LYS
SER
GLU
GLU
ALA
PRO
PRO
PRO
GLN
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THR
GLU
GLU
VAL
GLY
ILE
VAL
THR
LEU
GLU
ALA
GLN
THR
VAL

T26
L27
N28
T29
P32
F38
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S89
T90
Q91
E92
Q93
R96
V101
S107

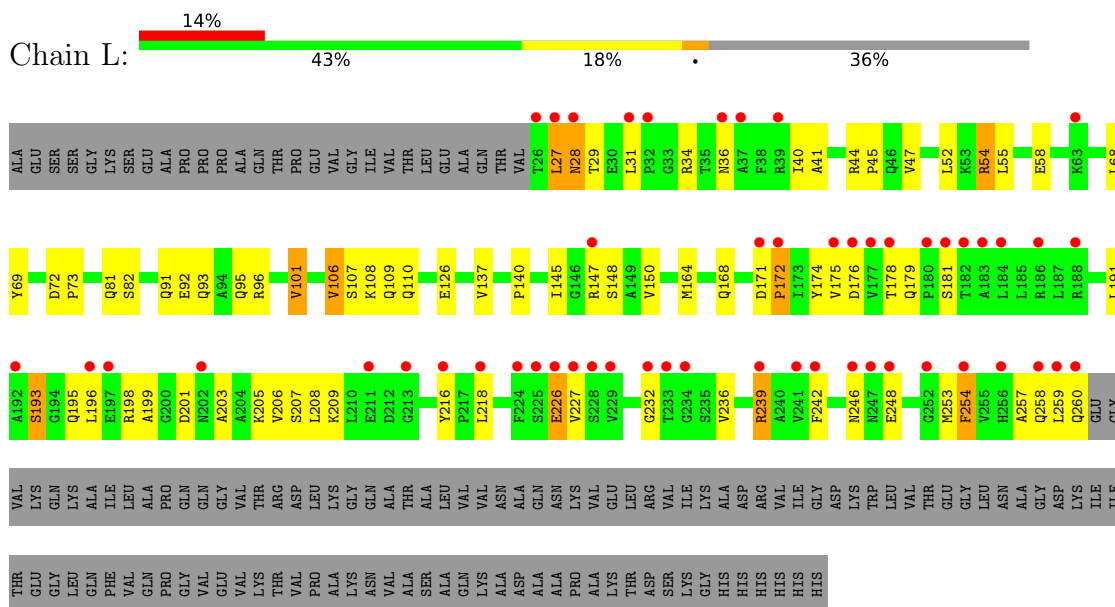
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Q109
Q110
Y118
L119
Q120
S121
V137
L138
S139
P140
R144
R147
M164
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I173
T178
Q179
P180
N181
S181
T182
L185
R188
R189
E190
L191
A192
S193
G194
Q195
L196
E197
R198
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K205
V206
S207
L208
K209
D212
G213
S214
V217



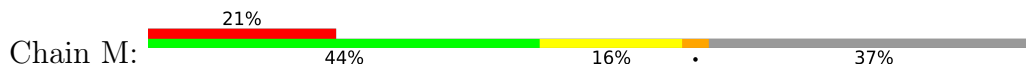
- Molecule 1: Multidrug resistance protein mexA

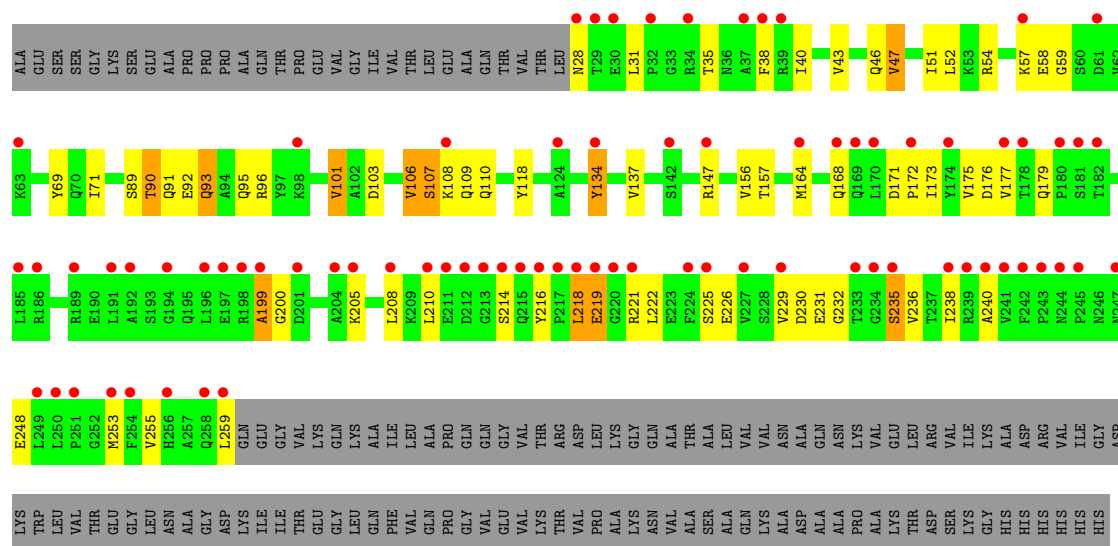


- Molecule 1: Multidrug resistance protein mexA



- Molecule 1: Multidrug resistance protein mexA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.03Å 180.35Å 214.23Å 90.00° 106.99° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.40) 99.8 (40.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.258 , 0.282 0.253 , 0.279	Depositor DCC
R_{free} test set	18428 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23655	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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

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	0.98	1/1840 (0.1%)	1.12	4/2495 (0.2%)
1	B	1.42	12/1827 (0.7%)	1.41	21/2478 (0.8%)
1	C	1.29	5/1909 (0.3%)	1.27	13/2588 (0.5%)
1	D	1.49	8/1827 (0.4%)	1.44	21/2478 (0.8%)
1	E	1.30	4/1953 (0.2%)	1.30	15/2648 (0.6%)
1	F	1.27	4/1812 (0.2%)	1.31	16/2457 (0.7%)
1	G	0.92	2/1843 (0.1%)	1.04	3/2500 (0.1%)
1	H	1.07	1/1870 (0.1%)	1.14	4/2537 (0.2%)
1	I	1.27	6/1827 (0.3%)	1.31	14/2478 (0.6%)
1	J	1.07	4/1827 (0.2%)	1.15	7/2478 (0.3%)
1	K	1.04	4/1803 (0.2%)	1.12	6/2445 (0.2%)
1	L	1.07	2/1827 (0.1%)	1.16	5/2478 (0.2%)
1	M	0.78	0/1803	1.00	2/2445 (0.1%)
All	All	1.17	53/23968 (0.2%)	1.22	131/32505 (0.4%)

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	ASN	C-O	18.19	1.45	1.24
1	B	55	LEU	N-CA	9.28	1.58	1.46
1	C	55	LEU	N-CA	8.55	1.57	1.46
1	I	55	LEU	N-CA	8.51	1.57	1.46
1	D	55	LEU	N-CA	7.56	1.55	1.46

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	ASN	N-CA-C	-13.20	87.38	108.90
1	B	246	ASN	CA-C-N	-13.19	96.36	121.54
1	B	246	ASN	C-N-CA	-13.19	96.36	121.54
1	I	172	PRO	N-CA-C	-11.77	92.90	111.03
1	F	246	ASN	CA-C-N	-11.21	105.88	122.24

There are no chirality outliers.

There are no planarity outliers.

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	1816	0	1816	57	0
1	B	1803	0	1807	50	0
1	C	1885	0	1902	56	0
1	D	1803	0	1807	42	0
1	E	1928	0	1941	56	0
1	F	1788	0	1789	45	0
1	G	1819	0	1822	39	0
1	H	1846	0	1849	28	0
1	I	1803	0	1807	42	0
1	J	1803	0	1807	42	0
1	K	1779	0	1781	56	0
1	L	1803	0	1807	55	0
1	M	1779	0	1781	45	0
All	All	23655	0	23716	562	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 12.

The worst 5 of 562 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:C:54:ARG:HG3	1:C:54:ARG:HH11	1.20	1.05
1:H:34:ARG:HG2	1:H:34:ARG:HH11	1.15	1.04
1:I:178:THR:HG22	1:I:237:THR:OG1	1.58	1.02
1:B:90:THR:HG23	1:B:118:TYR:HA	1.41	0.99
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.28	0.99

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	235/369 (64%)	213 (91%)	19 (8%)	3 (1%)	9	14
1	B	233/369 (63%)	216 (93%)	13 (6%)	4 (2%)	7	10
1	C	244/369 (66%)	236 (97%)	5 (2%)	3 (1%)	10	16
1	D	233/369 (63%)	222 (95%)	9 (4%)	2 (1%)	14	22
1	E	250/369 (68%)	232 (93%)	10 (4%)	8 (3%)	3	3
1	F	231/369 (63%)	211 (91%)	17 (7%)	3 (1%)	9	14
1	G	235/369 (64%)	226 (96%)	7 (3%)	2 (1%)	14	22
1	H	239/369 (65%)	228 (95%)	9 (4%)	2 (1%)	16	25
1	I	233/369 (63%)	228 (98%)	2 (1%)	3 (1%)	9	14
1	J	233/369 (63%)	225 (97%)	6 (3%)	2 (1%)	14	22
1	K	230/369 (62%)	208 (90%)	18 (8%)	4 (2%)	7	10
1	L	233/369 (63%)	216 (93%)	16 (7%)	1 (0%)	30	43
1	M	230/369 (62%)	204 (89%)	19 (8%)	7 (3%)	3	3
All	All	3059/4797 (64%)	2865 (94%)	150 (5%)	44 (1%)	9	13

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	VAL
1	E	267	ALA
1	F	29	THR
1	K	194	GLY
1	A	176	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	191/295 (65%)	170 (89%)	21 (11%)	6	9
1	B	190/295 (64%)	178 (94%)	12 (6%)	16	29
1	C	199/295 (68%)	187 (94%)	12 (6%)	17	31
1	D	190/295 (64%)	175 (92%)	15 (8%)	11	19
1	E	203/295 (69%)	182 (90%)	21 (10%)	7	11
1	F	188/295 (64%)	175 (93%)	13 (7%)	14	24
1	G	192/295 (65%)	175 (91%)	17 (9%)	9	15
1	H	195/295 (66%)	180 (92%)	15 (8%)	12	20
1	I	190/295 (64%)	179 (94%)	11 (6%)	18	32
1	J	190/295 (64%)	183 (96%)	7 (4%)	30	51
1	K	187/295 (63%)	175 (94%)	12 (6%)	16	28
1	L	190/295 (64%)	175 (92%)	15 (8%)	11	19
1	M	187/295 (63%)	172 (92%)	15 (8%)	11	19
All	All	2492/3835 (65%)	2306 (92%)	186 (8%)	12	21

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	89	SER
1	J	260	GLN
1	H	193	SER
1	I	101	VAL
1	K	122	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	84	GLN
1	M	169	GLN
1	I	215	GLN
1	M	168	GLN
1	L	168	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	237/369 (64%)	1.51	64 (27%) 1 1	41, 73, 122, 134	0
1	B	235/369 (63%)	0.60	23 (9%) 13 10	30, 51, 97, 109	0
1	C	246/369 (66%)	0.62	26 (10%) 11 8	29, 51, 92, 110	0
1	D	235/369 (63%)	0.34	16 (6%) 23 20	32, 46, 90, 101	0
1	E	252/369 (68%)	0.77	31 (12%) 8 6	35, 56, 112, 139	0
1	F	233/369 (63%)	0.72	30 (12%) 7 5	36, 56, 99, 106	0
1	G	237/369 (64%)	1.15	45 (18%) 3 2	46, 77, 118, 139	0
1	H	241/369 (65%)	0.89	26 (10%) 11 8	50, 68, 97, 114	0
1	I	235/369 (63%)	0.47	22 (9%) 14 11	35, 52, 95, 105	0
1	J	235/369 (63%)	0.98	51 (21%) 2 2	39, 58, 120, 125	0
1	K	232/369 (62%)	1.13	57 (24%) 2 1	41, 68, 116, 128	0
1	L	235/369 (63%)	1.14	52 (22%) 2 2	45, 69, 113, 120	0
1	M	232/369 (62%)	1.81	78 (33%) 1 1	56, 88, 150, 157	0
All	All	3085/4797 (64%)	0.93	521 (16%) 4 3	29, 64, 118, 157	0

The worst 5 of 521 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	LEU	11.8
1	L	27	LEU	11.6
1	A	227	VAL	11.5
1	E	274	GLY	11.3
1	G	25	VAL	11.0

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.