



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:54 AM GMT

PDB ID : 2V50  
Title : THE MISSING PART OF THE BACTERIAL MEXAB-OPRM SYSTEM:  
STRUCTURAL DETERMINATION OF THE MULTIDRUG EXPORTER  
MEXB  
Authors : Sennhauser, G.; Bukowska, M.A.; Gruetter, M.G.  
Deposited on : 2008-10-01  
Resolution : 3.00 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](mailto: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.

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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

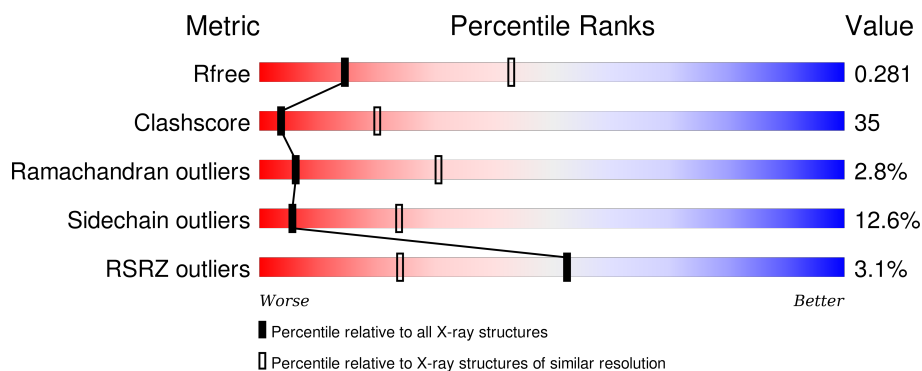
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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  $\geq 3$ , 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	1052	<div> <div>37%</div> <div>46%</div> <div>12%</div> <div>• •</div> </div>
1	B	1052	<div> <div>2%</div> <div>46%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>
1	C	1052	<div> <div>4%</div> <div>46%</div> <div>45%</div> <div>7%</div> <div>•</div> </div>
1	D	1052	<div> <div>2%</div> <div>38%</div> <div>46%</div> <div>11%</div> <div>• 5%</div> </div>
1	E	1052	<div> <div>4%</div> <div>44%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	1052	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	B	2032	-	-	-	X
2	LMT	B	2033	-	-	-	X
2	LMT	E	2032	-	-	-	X
2	LMT	E	2033	-	-	-	X

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 46628 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 MEXB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1005	Total	C	N	O	S	6	0	0
			7634	4920	1265	1410	39			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	12	0	0
			7812	5027	1298	1447	40			
1	D	998	Total	C	N	O	S	0	0	0
			7582	4888	1255	1399	40			
1	E	1012	Total	C	N	O	S	0	0	0
			7696	4956	1279	1421	40			
1	F	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			

There are 36 discrepancies between the modelled and reference sequences:

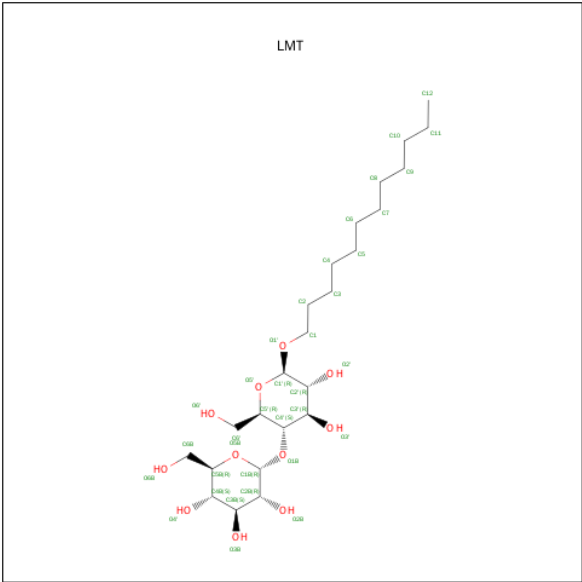
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	EXPRESSION TAG	UNP P52002
A	1048	HIS	-	EXPRESSION TAG	UNP P52002
A	1049	HIS	-	EXPRESSION TAG	UNP P52002
A	1050	HIS	-	EXPRESSION TAG	UNP P52002
A	1051	HIS	-	EXPRESSION TAG	UNP P52002
A	1052	HIS	-	EXPRESSION TAG	UNP P52002
B	1047	HIS	-	EXPRESSION TAG	UNP P52002
B	1048	HIS	-	EXPRESSION TAG	UNP P52002
B	1049	HIS	-	EXPRESSION TAG	UNP P52002
B	1050	HIS	-	EXPRESSION TAG	UNP P52002
B	1051	HIS	-	EXPRESSION TAG	UNP P52002
B	1052	HIS	-	EXPRESSION TAG	UNP P52002
C	1047	HIS	-	EXPRESSION TAG	UNP P52002
C	1048	HIS	-	EXPRESSION TAG	UNP P52002
C	1049	HIS	-	EXPRESSION TAG	UNP P52002
C	1050	HIS	-	EXPRESSION TAG	UNP P52002
C	1051	HIS	-	EXPRESSION TAG	UNP P52002

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1052	HIS	-	EXPRESSION TAG	UNP P52002
D	1047	HIS	-	EXPRESSION TAG	UNP P52002
D	1048	HIS	-	EXPRESSION TAG	UNP P52002
D	1049	HIS	-	EXPRESSION TAG	UNP P52002
D	1050	HIS	-	EXPRESSION TAG	UNP P52002
D	1051	HIS	-	EXPRESSION TAG	UNP P52002
D	1052	HIS	-	EXPRESSION TAG	UNP P52002
E	1047	HIS	-	EXPRESSION TAG	UNP P52002
E	1048	HIS	-	EXPRESSION TAG	UNP P52002
E	1049	HIS	-	EXPRESSION TAG	UNP P52002
E	1050	HIS	-	EXPRESSION TAG	UNP P52002
E	1051	HIS	-	EXPRESSION TAG	UNP P52002
E	1052	HIS	-	EXPRESSION TAG	UNP P52002
F	1047	HIS	-	EXPRESSION TAG	UNP P52002
F	1048	HIS	-	EXPRESSION TAG	UNP P52002
F	1049	HIS	-	EXPRESSION TAG	UNP P52002
F	1050	HIS	-	EXPRESSION TAG	UNP P52002
F	1051	HIS	-	EXPRESSION TAG	UNP P52002
F	1052	HIS	-	EXPRESSION TAG	UNP P52002

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		

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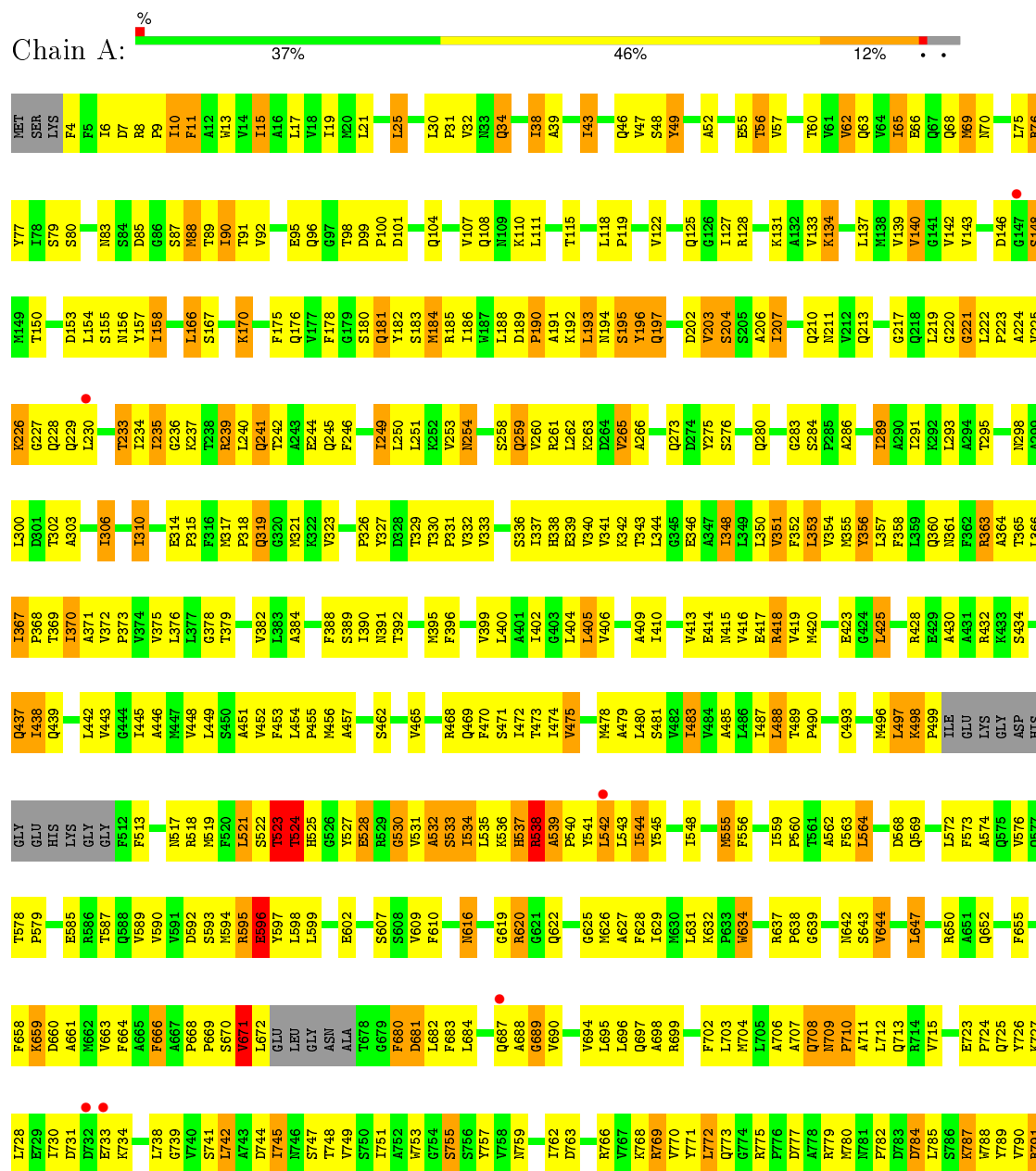
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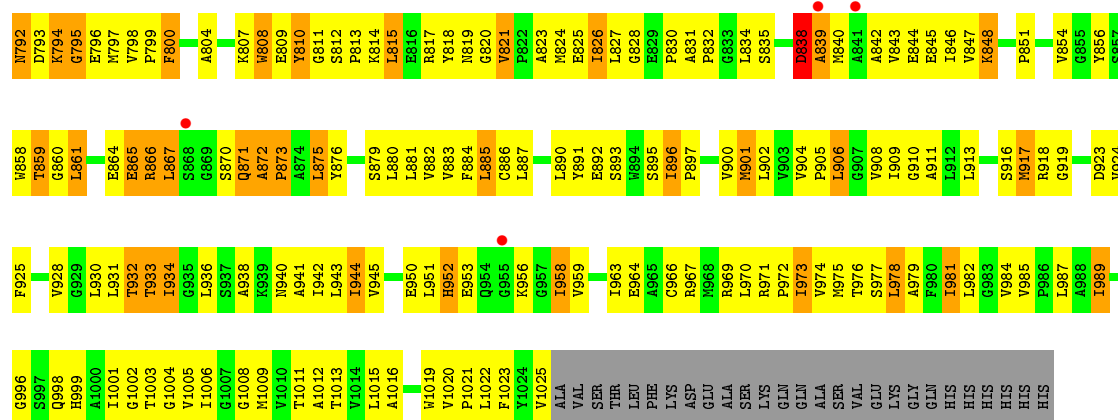
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		

### 3 Residue-property plots

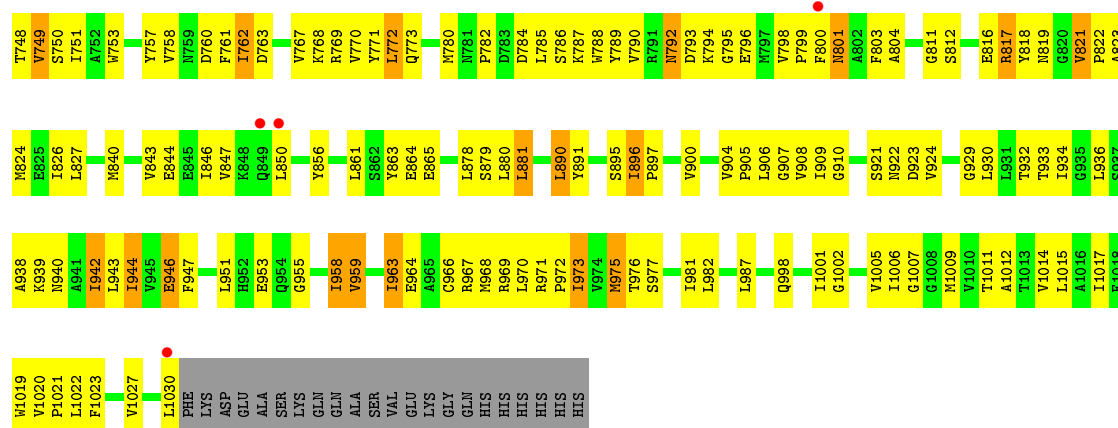
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: MULTIDRUG RESISTANCE PROTEIN MEXB

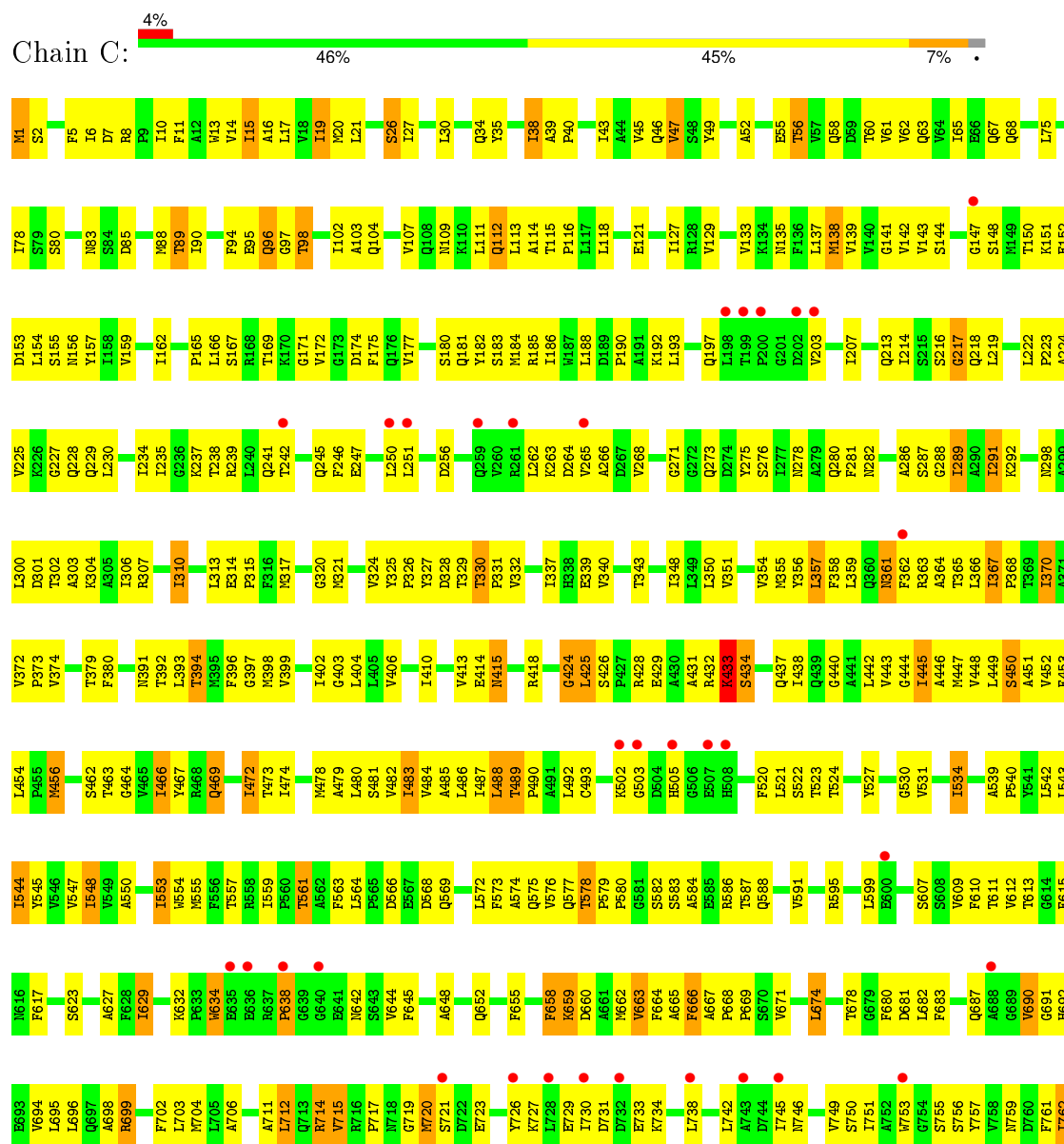


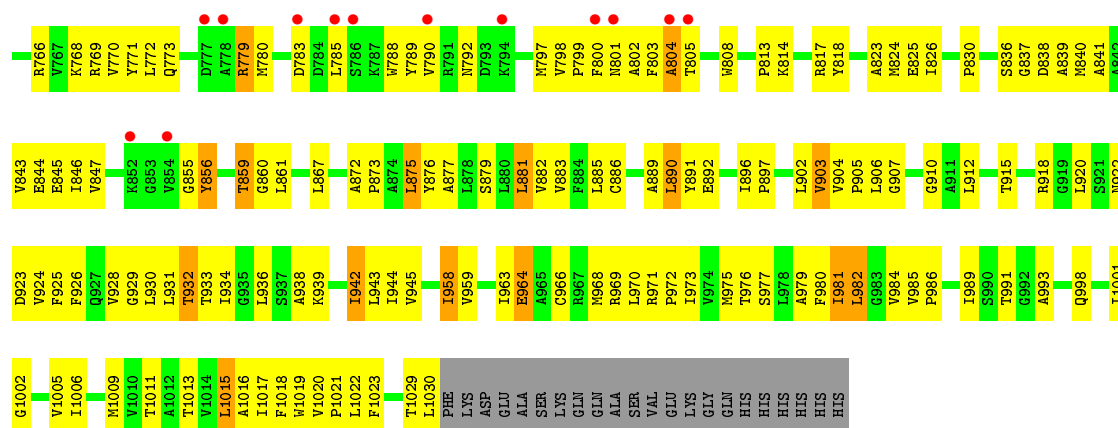




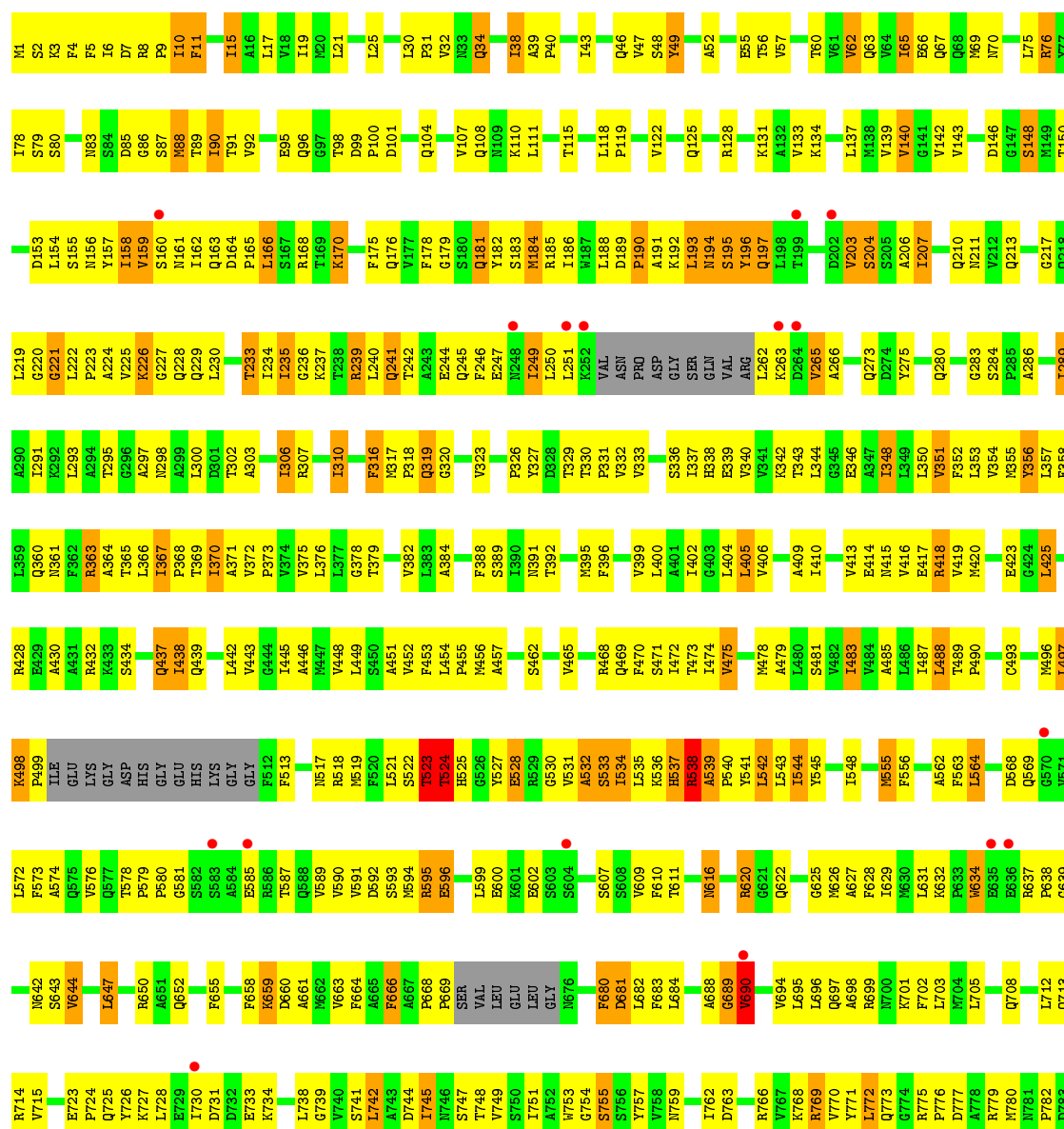


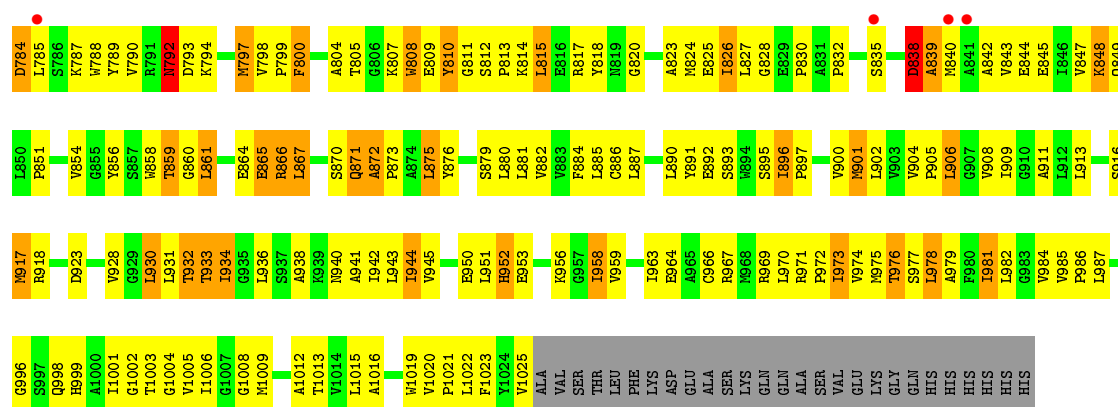
### • Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB



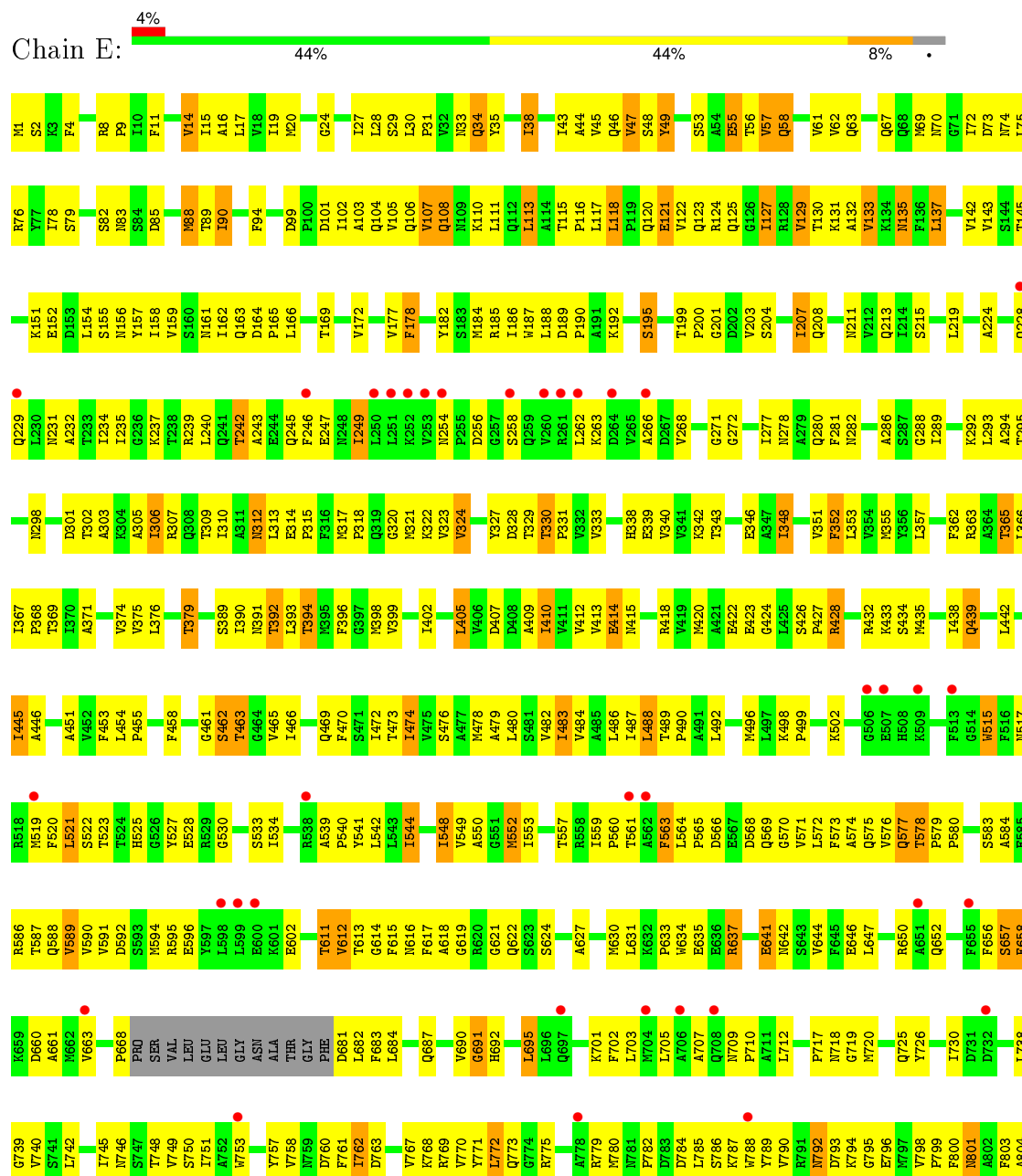


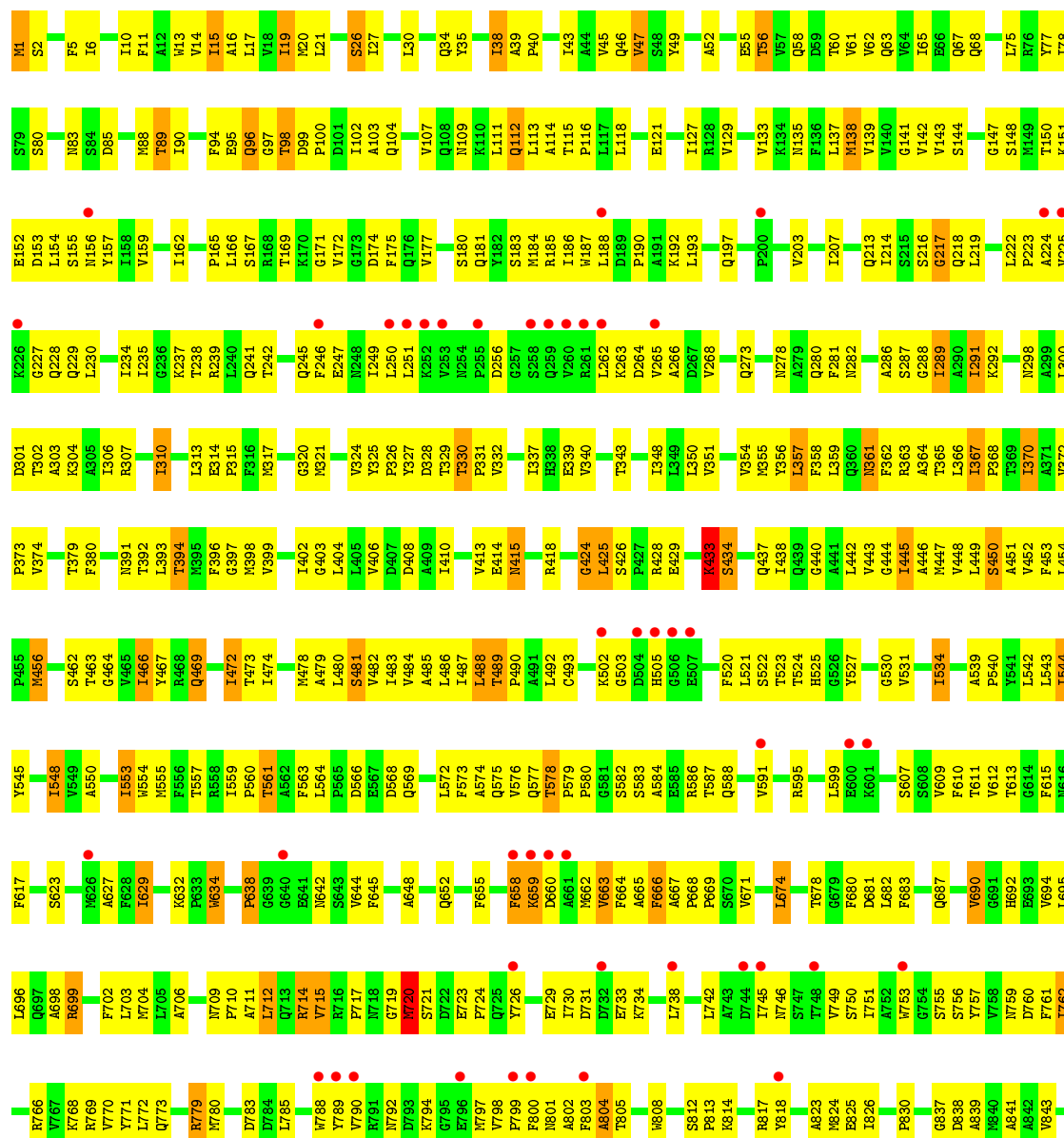
## • Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB





## • Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB





I1012	I846
I1013	I847
I1014	I855
I1015	I856
A1016	I859
I1017	I860
F1018	I867
I1019	A872
V1020	P873
P1021	A874
L1022	I875
F1023	I876
I1029	I877
L1030	I878
PHE	I879
LYS	I880
ASP	I881
GLU	I882
ALA	I883
SER	I884
LYS	I885
GLN	I886
GLN	I889
ALA	I890
SER	I891
VAL	I892
GLU	I896
LYS	I897
GLY	I902
GLN	I903
HIS	I904
HIS	I905
HIS	I906
HIS	I907
HIS	I910
HIS	I911
	I912
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	I1001
	I1002
	I1005
	I1006
	I1009
	I1010
	I1011

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.05Å 134.58Å 151.02Å 86.99° 69.70° 88.16°	Depositor
Resolution (Å)	49.76 – 3.00 49.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.76-3.00) 95.2 (49.76-3.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.242 , 0.287 0.237 , 0.281	Depositor DCC
$R_{free}$ test set	3536 reflections (2.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 176904 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	46628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.30	0/7789	0.50	0/10588
1	B	0.30	0/7971	0.46	0/10833
1	C	0.27	0/7971	0.45	0/10833
1	D	0.30	0/7735	0.50	0/10510
1	E	0.29	0/7851	0.47	0/10666
1	F	0.28	0/7971	0.45	0/10833
All	All	0.29	0/47288	0.47	0/64263

There are no bond length outliers.

There are no bond angle outliers.

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	7634	0	7765	689	0
1	B	7812	0	7944	541	0
1	C	7812	0	7944	509	0
1	D	7582	0	7716	665	0
1	E	7696	0	7832	528	0
1	F	7812	0	7944	509	0
2	A	35	0	46	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	105	0	138	17	0
2	D	35	0	46	5	0
2	E	105	0	138	22	0
All	All	46628	0	47513	3338	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 35.

The worst 5 of 3338 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:76:ARG:HH11	1:A:76:ARG:HG2	1.09	1.13
1:B:43:ILE:HG21	1:B:107:VAL:HG11	1.30	1.12
1:A:375:VAL:HG21	1:A:405:LEU:HG	1.33	1.11
1:C:699:ARG:HH11	1:C:699:ARG:HG3	1.09	1.10
1:F:699:ARG:HH11	1:F:699:ARG:HG3	1.08	1.09

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	999/1052 (95%)	830 (83%)	123 (12%)	46 (5%)	3	18
1	B	1028/1052 (98%)	863 (84%)	147 (14%)	18 (2%)	11	45
1	C	1028/1052 (98%)	859 (84%)	143 (14%)	26 (2%)	7	34
1	D	990/1052 (94%)	820 (83%)	132 (13%)	38 (4%)	4	22
1	E	1006/1052 (96%)	847 (84%)	141 (14%)	18 (2%)	11	45
1	F	1028/1052 (98%)	866 (84%)	136 (13%)	26 (2%)	7	34
All	All	6079/6312 (96%)	5085 (84%)	822 (14%)	172 (3%)	6	30



5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	134	LYS
1	A	203	VAL
1	A	204	SER
1	A	498	LYS

### 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	823/860 (96%)	697 (85%)	126 (15%)	3	16
1	B	841/860 (98%)	736 (88%)	105 (12%)	6	24
1	C	841/860 (98%)	755 (90%)	86 (10%)	9	33
1	D	816/860 (95%)	695 (85%)	121 (15%)	4	17
1	E	829/860 (96%)	727 (88%)	102 (12%)	6	25
1	F	841/860 (98%)	751 (89%)	90 (11%)	8	31
All	All	4991/5160 (97%)	4361 (87%)	630 (13%)	5	24

5 of 630 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	578	THR
1	D	249	ILE
1	F	450	SER
1	C	704	MET
1	D	15	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	437	GLN
1	D	213	GLN

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Mol	Chain	Res	Type
1	F	282	ASN
1	C	469	GLN
1	D	68	GLN

### 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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LMT	A	2026	-	36,36,36	0.56	0	47,47,47	1.54	7 (14%)
2	LMT	B	2031	-	36,36,36	0.95	2 (5%)	47,47,47	1.43	9 (19%)
2	LMT	B	2032	-	36,36,36	0.73	1 (2%)	47,47,47	2.01	9 (19%)
2	LMT	B	2033	-	36,36,36	1.15	3 (8%)	47,47,47	3.58	19 (40%)
2	LMT	D	2026	-	36,36,36	0.70	1 (2%)	47,47,47	1.85	8 (17%)
2	LMT	E	2031	-	36,36,36	0.86	1 (2%)	47,47,47	1.82	9 (19%)
2	LMT	E	2032	-	36,36,36	0.60	1 (2%)	47,47,47	1.42	5 (10%)
2	LMT	E	2033	-	36,36,36	1.07	3 (8%)	47,47,47	3.49	19 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	A	2026	-	-	1/21/61/61	0/2/2/2
2	LMT	B	2031	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2032	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2033	-	-	1/21/61/61	0/2/2/2
2	LMT	D	2026	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2031	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2032	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2033	-	-	1/21/61/61	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2033	LMT	O5'-C5'	2.05	1.49	1.44
2	B	2033	LMT	O5'-C5'	2.06	1.49	1.44
2	B	2031	LMT	O1B-C1B	2.06	1.47	1.41
2	E	2033	LMT	O1B-C1B	2.16	1.47	1.41
2	E	2032	LMT	O1'-C1'	2.32	1.44	1.40

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2033	LMT	C1B-O1B-C4'	-9.52	93.14	118.01
2	E	2033	LMT	C1B-O1B-C4'	-9.16	94.06	118.01
2	B	2033	LMT	C3'-C4'-C5'	-7.97	92.81	110.84
2	E	2033	LMT	C3'-C4'-C5'	-7.91	92.95	110.84
2	B	2032	LMT	C1-O1'-C1'	-7.22	101.33	113.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2026	LMT	C1-O1'-C1'-O5'
2	E	2033	LMT	C1-O1'-C1'-O5'
2	B	2033	LMT	C1-O1'-C1'-O5'

There are no ring outliers.

8 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2026	LMT	10	0
2	B	2031	LMT	5	0
2	B	2032	LMT	4	0
2	B	2033	LMT	8	0
2	D	2026	LMT	5	0
2	E	2031	LMT	4	0
2	E	2032	LMT	8	0
2	E	2033	LMT	10	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1004/1052 (95%)	-0.23	10 (0%)	84 60	54, 91, 132, 178	0
1	B	1030/1052 (97%)	-0.11	26 (2%)	61 30	53, 91, 143, 188	0
1	C	1028/1052 (97%)	-0.04	46 (4%)	37 15	58, 101, 178, 238	0
1	D	998/1052 (94%)	-0.26	20 (2%)	68 39	58, 91, 134, 179	0
1	E	1012/1052 (96%)	-0.13	43 (4%)	40 16	55, 93, 143, 189	0
1	F	1030/1052 (97%)	-0.06	47 (4%)	36 14	59, 100, 177, 238	0
All	All	6102/6312 (96%)	-0.14	192 (3%)	52 24	53, 94, 153, 238	0

The worst 5 of 192 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	803	PHE	7.8
1	E	260	VAL	6.8
1	C	778	ALA	6.2
1	E	251	LEU	6.1
1	F	753	TRP	5.6

### 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

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	LMT	B	2033	35/35	0.72	0.42	3.49	100,155,176,183	0
2	LMT	E	2033	35/35	0.76	0.33	2.43	111,146,174,179	0
2	LMT	B	2032	35/35	0.93	0.25	2.22	52,70,157,169	0
2	LMT	E	2032	35/35	0.93	0.23	2.19	66,90,115,128	0
2	LMT	E	2031	35/35	0.85	0.23	1.97	72,95,121,130	0
2	LMT	A	2026	35/35	0.90	0.21	0.66	80,110,145,173	0
2	LMT	B	2031	35/35	0.90	0.19	0.05	59,82,109,114	0
2	LMT	D	2026	35/35	0.91	0.16	-1.02	75,113,140,142	0

## 6.5 Other polymers

There are no such residues in this entry.