wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 07:05 pm GMT

PDB ID	:	5AA3
Title	:	Crystal structure of MltF from Pseudomonas aeruginosa in the presence of tetrasaccharide and tetrapeptide
Authors	:	Dominguez-Gil, T.; Acebron, I.; Hermoso, J.A.
Deposited on	:	2015-07-23
Resolution	:	3.20 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 (i) 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 (1)) were used in the production of this report:

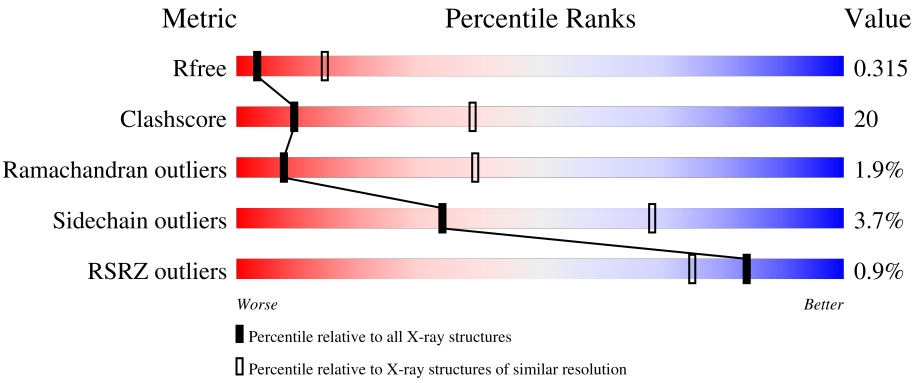
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	499	58% 23% 16%
1	B	499	56% 26% 16%
1	C	499	56% 25% 16%
1	D	499	56% 23% 17%
1	E	499	58% 25% 16%

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Mol	Chain	Length	Quality of chain
1	F	499	55% 26% 17%
1	G	499	56% 24% 17%
1	H	499	59% 22% 17%
1	I	499	52% 28% 16%
1	J	499	53% 26% 17%
1	K	499	57% 23% 16%
1	L	499	51% 30% 16%

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	GLU	A	501	-	-	X	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40234 atoms, of which 8 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 MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	2	0
			3361	2121	598	633	9			
1	B	417	Total	C	N	O	S	0	1	0
			3351	2112	597	633	9			
1	C	418	Total	C	N	O	S	0	2	0
			3370	2126	599	636	9			
1	D	415	Total	C	N	O	S	0	1	0
			3333	2102	594	628	9			
1	E	418	Total	C	N	O	S	0	1	0
			3358	2117	599	633	9			
1	F	416	Total	C	N	O	S	0	2	0
			3351	2112	598	632	9			
1	G	416	Total	C	N	O	S	0	1	0
			3342	2107	596	630	9			
1	H	415	Total	C	N	O	S	0	1	0
			3333	2102	594	628	9			
1	I	418	Total	C	N	O	S	0	1	0
			3360	2118	599	634	9			
1	J	416	Total	C	N	O	S	0	1	0
			3342	2107	596	630	9			
1	K	417	Total	C	N	O	S	0	1	0
			3349	2112	597	631	9			
1	L	419	Total	C	N	O	S	0	1	0
			3366	2122	600	634	10			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q9HXN1
A	-7	ALA	-	expression tag	UNP Q9HXN1
A	-6	PRO	-	expression tag	UNP Q9HXN1
A	-5	SER	-	expression tag	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ARG	-	expression tag	UNP Q9HXN1
A	-3	LEU	-	expression tag	UNP Q9HXN1
A	-2	CYS	-	expression tag	UNP Q9HXN1
A	-1	VAL	-	expression tag	UNP Q9HXN1
A	0	TYR	-	expression tag	UNP Q9HXN1
A	1	CYS	-	expression tag	UNP Q9HXN1
A	2	ALA	-	expression tag	UNP Q9HXN1
A	3	ASP	-	expression tag	UNP Q9HXN1
A	4	VAL	-	expression tag	UNP Q9HXN1
A	5	CYS	-	expression tag	UNP Q9HXN1
A	6	PRO	-	expression tag	UNP Q9HXN1
A	7	ASP	-	expression tag	UNP Q9HXN1
A	302	LYS	LEU	conflict	UNP Q9HXN1
B	-8	MET	-	expression tag	UNP Q9HXN1
B	-7	ALA	-	expression tag	UNP Q9HXN1
B	-6	PRO	-	expression tag	UNP Q9HXN1
B	-5	SER	-	expression tag	UNP Q9HXN1
B	-4	ARG	-	expression tag	UNP Q9HXN1
B	-3	LEU	-	expression tag	UNP Q9HXN1
B	-2	CYS	-	expression tag	UNP Q9HXN1
B	-1	VAL	-	expression tag	UNP Q9HXN1
B	0	TYR	-	expression tag	UNP Q9HXN1
B	1	CYS	-	expression tag	UNP Q9HXN1
B	2	ALA	-	expression tag	UNP Q9HXN1
B	3	ASP	-	expression tag	UNP Q9HXN1
B	4	VAL	-	expression tag	UNP Q9HXN1
B	5	CYS	-	expression tag	UNP Q9HXN1
B	6	PRO	-	expression tag	UNP Q9HXN1
B	7	ASP	-	expression tag	UNP Q9HXN1
B	302	LYS	LEU	conflict	UNP Q9HXN1
C	-8	MET	-	expression tag	UNP Q9HXN1
C	-7	ALA	-	expression tag	UNP Q9HXN1
C	-6	PRO	-	expression tag	UNP Q9HXN1
C	-5	SER	-	expression tag	UNP Q9HXN1
C	-4	ARG	-	expression tag	UNP Q9HXN1
C	-3	LEU	-	expression tag	UNP Q9HXN1
C	-2	CYS	-	expression tag	UNP Q9HXN1
C	-1	VAL	-	expression tag	UNP Q9HXN1
C	0	TYR	-	expression tag	UNP Q9HXN1
C	1	CYS	-	expression tag	UNP Q9HXN1
C	2	ALA	-	expression tag	UNP Q9HXN1
C	3	ASP	-	expression tag	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	VAL	-	expression tag	UNP Q9HXN1
C	5	CYS	-	expression tag	UNP Q9HXN1
C	6	PRO	-	expression tag	UNP Q9HXN1
C	7	ASP	-	expression tag	UNP Q9HXN1
C	302	LYS	LEU	conflict	UNP Q9HXN1
D	-8	MET	-	expression tag	UNP Q9HXN1
D	-7	ALA	-	expression tag	UNP Q9HXN1
D	-6	PRO	-	expression tag	UNP Q9HXN1
D	-5	SER	-	expression tag	UNP Q9HXN1
D	-4	ARG	-	expression tag	UNP Q9HXN1
D	-3	LEU	-	expression tag	UNP Q9HXN1
D	-2	CYS	-	expression tag	UNP Q9HXN1
D	-1	VAL	-	expression tag	UNP Q9HXN1
D	0	TYR	-	expression tag	UNP Q9HXN1
D	1	CYS	-	expression tag	UNP Q9HXN1
D	2	ALA	-	expression tag	UNP Q9HXN1
D	3	ASP	-	expression tag	UNP Q9HXN1
D	4	VAL	-	expression tag	UNP Q9HXN1
D	5	CYS	-	expression tag	UNP Q9HXN1
D	6	PRO	-	expression tag	UNP Q9HXN1
D	7	ASP	-	expression tag	UNP Q9HXN1
D	302	LYS	LEU	conflict	UNP Q9HXN1
E	-8	MET	-	expression tag	UNP Q9HXN1
E	-7	ALA	-	expression tag	UNP Q9HXN1
E	-6	PRO	-	expression tag	UNP Q9HXN1
E	-5	SER	-	expression tag	UNP Q9HXN1
E	-4	ARG	-	expression tag	UNP Q9HXN1
E	-3	LEU	-	expression tag	UNP Q9HXN1
E	-2	CYS	-	expression tag	UNP Q9HXN1
E	-1	VAL	-	expression tag	UNP Q9HXN1
E	0	TYR	-	expression tag	UNP Q9HXN1
E	1	CYS	-	expression tag	UNP Q9HXN1
E	2	ALA	-	expression tag	UNP Q9HXN1
E	3	ASP	-	expression tag	UNP Q9HXN1
E	4	VAL	-	expression tag	UNP Q9HXN1
E	5	CYS	-	expression tag	UNP Q9HXN1
E	6	PRO	-	expression tag	UNP Q9HXN1
E	7	ASP	-	expression tag	UNP Q9HXN1
E	302	LYS	LEU	conflict	UNP Q9HXN1
F	-8	MET	-	expression tag	UNP Q9HXN1
F	-7	ALA	-	expression tag	UNP Q9HXN1
F	-6	PRO	-	expression tag	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	SER	-	expression tag	UNP Q9HXN1
F	-4	ARG	-	expression tag	UNP Q9HXN1
F	-3	LEU	-	expression tag	UNP Q9HXN1
F	-2	CYS	-	expression tag	UNP Q9HXN1
F	-1	VAL	-	expression tag	UNP Q9HXN1
F	0	TYR	-	expression tag	UNP Q9HXN1
F	1	CYS	-	expression tag	UNP Q9HXN1
F	2	ALA	-	expression tag	UNP Q9HXN1
F	3	ASP	-	expression tag	UNP Q9HXN1
F	4	VAL	-	expression tag	UNP Q9HXN1
F	5	CYS	-	expression tag	UNP Q9HXN1
F	6	PRO	-	expression tag	UNP Q9HXN1
F	7	ASP	-	expression tag	UNP Q9HXN1
F	302	LYS	LEU	conflict	UNP Q9HXN1
G	-8	MET	-	expression tag	UNP Q9HXN1
G	-7	ALA	-	expression tag	UNP Q9HXN1
G	-6	PRO	-	expression tag	UNP Q9HXN1
G	-5	SER	-	expression tag	UNP Q9HXN1
G	-4	ARG	-	expression tag	UNP Q9HXN1
G	-3	LEU	-	expression tag	UNP Q9HXN1
G	-2	CYS	-	expression tag	UNP Q9HXN1
G	-1	VAL	-	expression tag	UNP Q9HXN1
G	0	TYR	-	expression tag	UNP Q9HXN1
G	1	CYS	-	expression tag	UNP Q9HXN1
G	2	ALA	-	expression tag	UNP Q9HXN1
G	3	ASP	-	expression tag	UNP Q9HXN1
G	4	VAL	-	expression tag	UNP Q9HXN1
G	5	CYS	-	expression tag	UNP Q9HXN1
G	6	PRO	-	expression tag	UNP Q9HXN1
G	7	ASP	-	expression tag	UNP Q9HXN1
G	302	LYS	LEU	conflict	UNP Q9HXN1
H	-8	MET	-	expression tag	UNP Q9HXN1
H	-7	ALA	-	expression tag	UNP Q9HXN1
H	-6	PRO	-	expression tag	UNP Q9HXN1
H	-5	SER	-	expression tag	UNP Q9HXN1
H	-4	ARG	-	expression tag	UNP Q9HXN1
H	-3	LEU	-	expression tag	UNP Q9HXN1
H	-2	CYS	-	expression tag	UNP Q9HXN1
H	-1	VAL	-	expression tag	UNP Q9HXN1
H	0	TYR	-	expression tag	UNP Q9HXN1
H	1	CYS	-	expression tag	UNP Q9HXN1
H	2	ALA	-	expression tag	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	3	ASP	-	expression tag	UNP Q9HXN1
H	4	VAL	-	expression tag	UNP Q9HXN1
H	5	CYS	-	expression tag	UNP Q9HXN1
H	6	PRO	-	expression tag	UNP Q9HXN1
H	7	ASP	-	expression tag	UNP Q9HXN1
H	302	LYS	LEU	conflict	UNP Q9HXN1
I	-8	MET	-	expression tag	UNP Q9HXN1
I	-7	ALA	-	expression tag	UNP Q9HXN1
I	-6	PRO	-	expression tag	UNP Q9HXN1
I	-5	SER	-	expression tag	UNP Q9HXN1
I	-4	ARG	-	expression tag	UNP Q9HXN1
I	-3	LEU	-	expression tag	UNP Q9HXN1
I	-2	CYS	-	expression tag	UNP Q9HXN1
I	-1	VAL	-	expression tag	UNP Q9HXN1
I	0	TYR	-	expression tag	UNP Q9HXN1
I	1	CYS	-	expression tag	UNP Q9HXN1
I	2	ALA	-	expression tag	UNP Q9HXN1
I	3	ASP	-	expression tag	UNP Q9HXN1
I	4	VAL	-	expression tag	UNP Q9HXN1
I	5	CYS	-	expression tag	UNP Q9HXN1
I	6	PRO	-	expression tag	UNP Q9HXN1
I	7	ASP	-	expression tag	UNP Q9HXN1
I	302	LYS	LEU	conflict	UNP Q9HXN1
J	-8	MET	-	expression tag	UNP Q9HXN1
J	-7	ALA	-	expression tag	UNP Q9HXN1
J	-6	PRO	-	expression tag	UNP Q9HXN1
J	-5	SER	-	expression tag	UNP Q9HXN1
J	-4	ARG	-	expression tag	UNP Q9HXN1
J	-3	LEU	-	expression tag	UNP Q9HXN1
J	-2	CYS	-	expression tag	UNP Q9HXN1
J	-1	VAL	-	expression tag	UNP Q9HXN1
J	0	TYR	-	expression tag	UNP Q9HXN1
J	1	CYS	-	expression tag	UNP Q9HXN1
J	2	ALA	-	expression tag	UNP Q9HXN1
J	3	ASP	-	expression tag	UNP Q9HXN1
J	4	VAL	-	expression tag	UNP Q9HXN1
J	5	CYS	-	expression tag	UNP Q9HXN1
J	6	PRO	-	expression tag	UNP Q9HXN1
J	7	ASP	-	expression tag	UNP Q9HXN1
J	302	LYS	LEU	conflict	UNP Q9HXN1
K	-8	MET	-	expression tag	UNP Q9HXN1
K	-7	ALA	-	expression tag	UNP Q9HXN1

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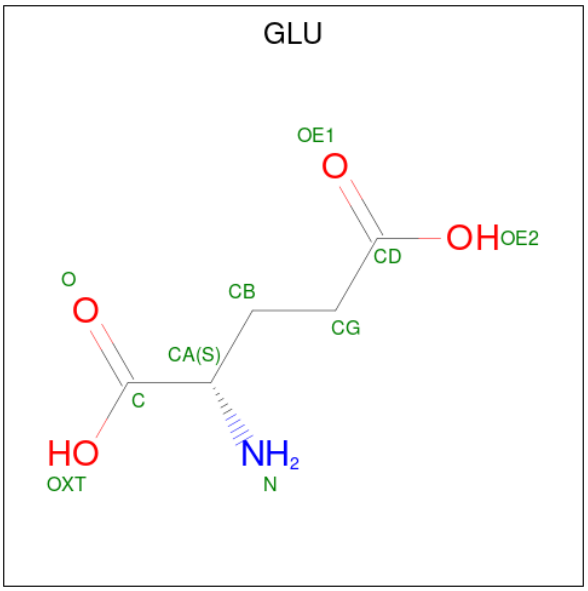
Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	PRO	-	expression tag	UNP Q9HXN1
K	-5	SER	-	expression tag	UNP Q9HXN1
K	-4	ARG	-	expression tag	UNP Q9HXN1
K	-3	LEU	-	expression tag	UNP Q9HXN1
K	-2	CYS	-	expression tag	UNP Q9HXN1
K	-1	VAL	-	expression tag	UNP Q9HXN1
K	0	TYR	-	expression tag	UNP Q9HXN1
K	1	CYS	-	expression tag	UNP Q9HXN1
K	2	ALA	-	expression tag	UNP Q9HXN1
K	3	ASP	-	expression tag	UNP Q9HXN1
K	4	VAL	-	expression tag	UNP Q9HXN1
K	5	CYS	-	expression tag	UNP Q9HXN1
K	6	PRO	-	expression tag	UNP Q9HXN1
K	7	ASP	-	expression tag	UNP Q9HXN1
K	302	LYS	LEU	conflict	UNP Q9HXN1
L	-8	MET	-	expression tag	UNP Q9HXN1
L	-7	ALA	-	expression tag	UNP Q9HXN1
L	-6	PRO	-	expression tag	UNP Q9HXN1
L	-5	SER	-	expression tag	UNP Q9HXN1
L	-4	ARG	-	expression tag	UNP Q9HXN1
L	-3	LEU	-	expression tag	UNP Q9HXN1
L	-2	CYS	-	expression tag	UNP Q9HXN1
L	-1	VAL	-	expression tag	UNP Q9HXN1
L	0	TYR	-	expression tag	UNP Q9HXN1
L	1	CYS	-	expression tag	UNP Q9HXN1
L	2	ALA	-	expression tag	UNP Q9HXN1
L	3	ASP	-	expression tag	UNP Q9HXN1
L	4	VAL	-	expression tag	UNP Q9HXN1
L	5	CYS	-	expression tag	UNP Q9HXN1
L	6	PRO	-	expression tag	UNP Q9HXN1
L	7	ASP	-	expression tag	UNP Q9HXN1
L	302	LYS	LEU	conflict	UNP Q9HXN1

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



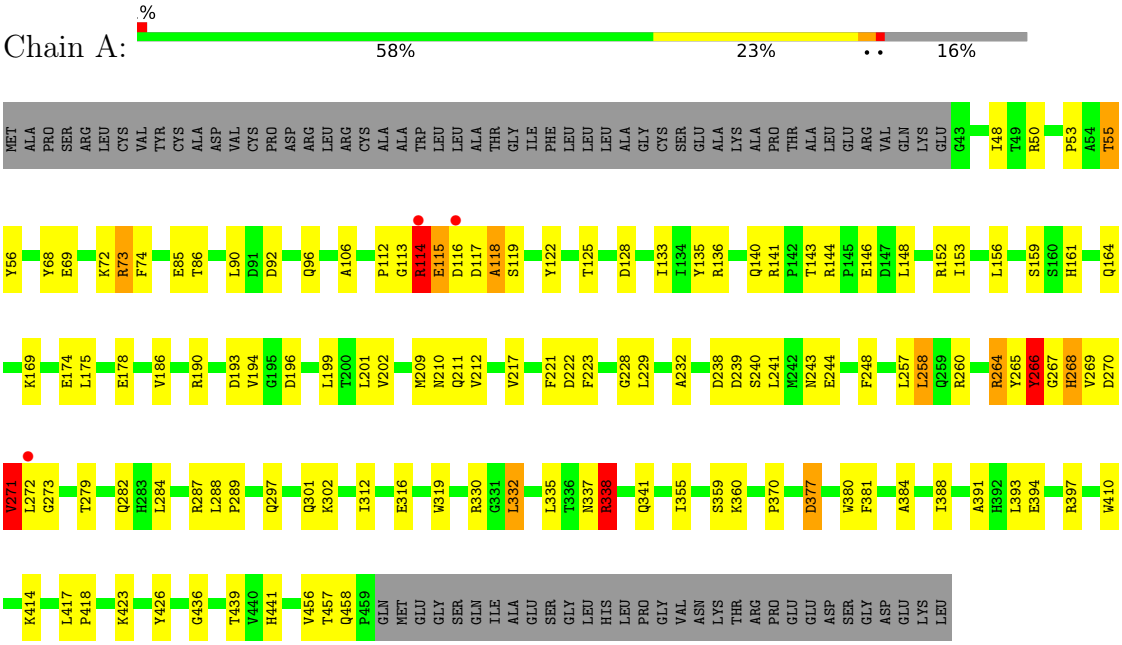
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			18	5	8	1	4		

3 Residue-property plots (i)

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.

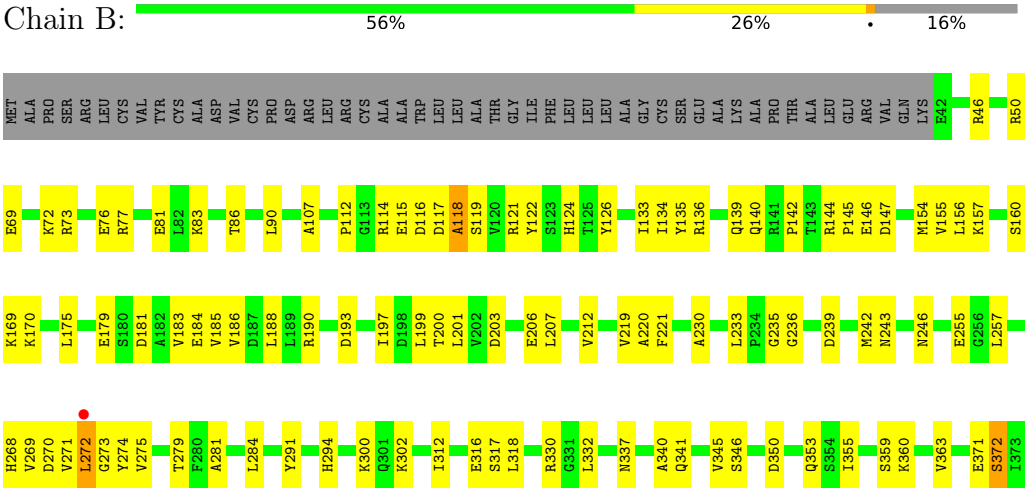
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

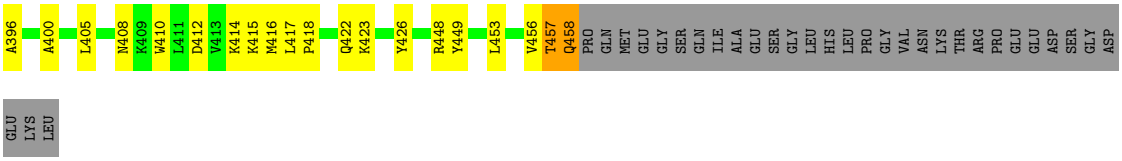
Chain A:



• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

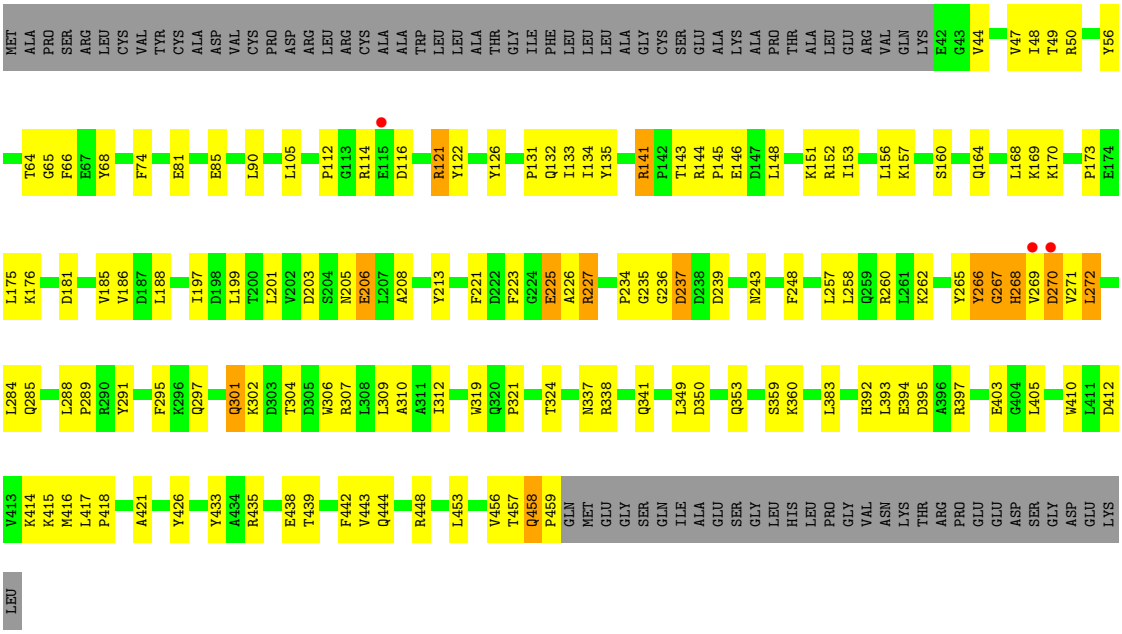
Chain B:





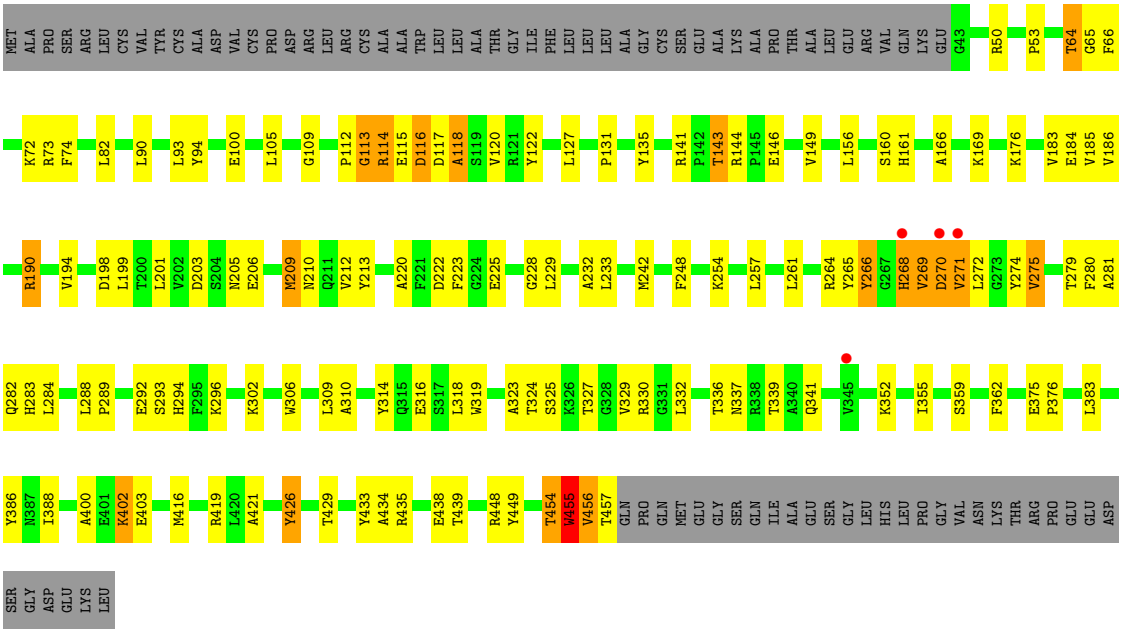
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain C:



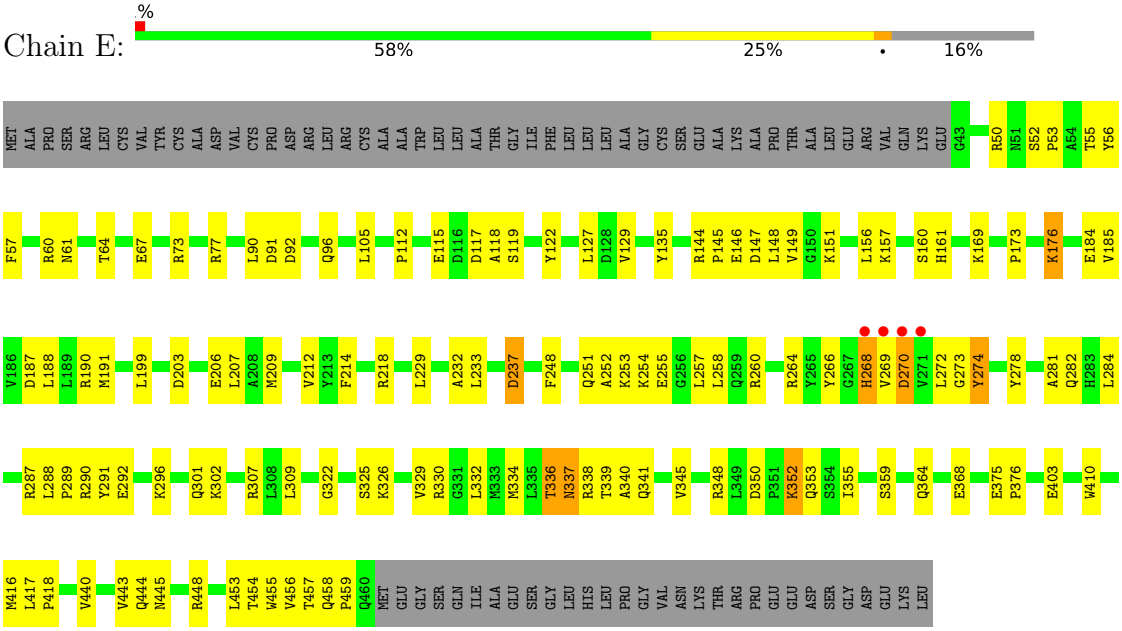
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain D:



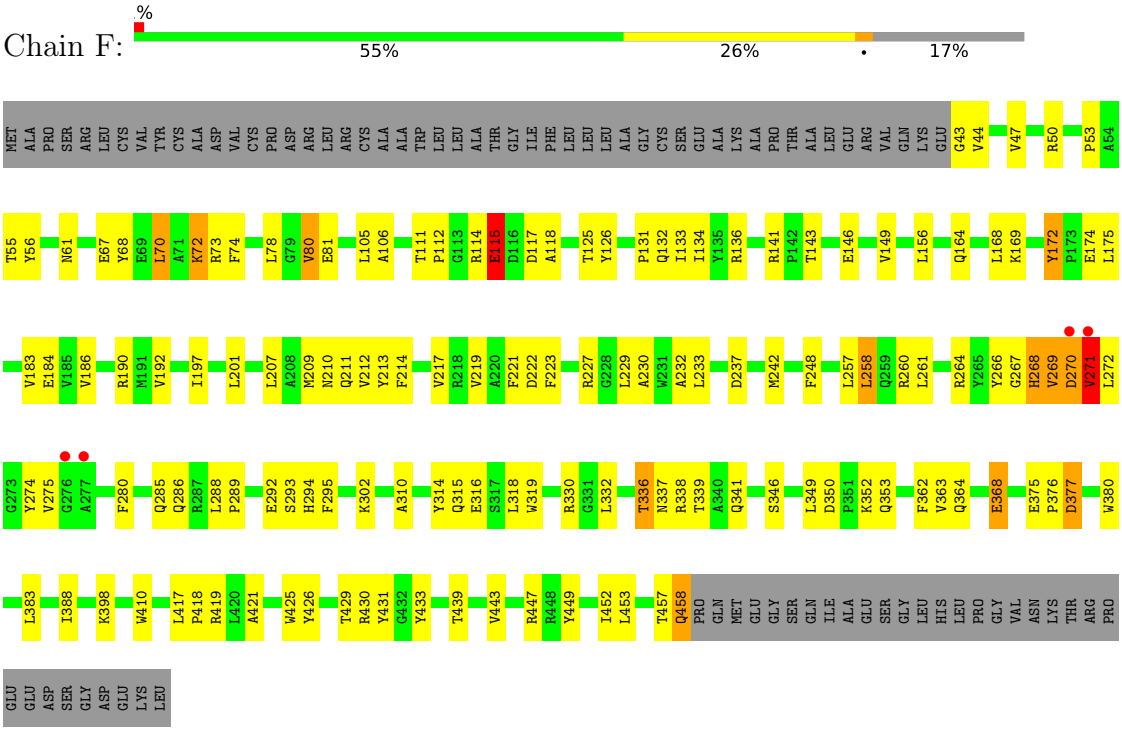
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain E:



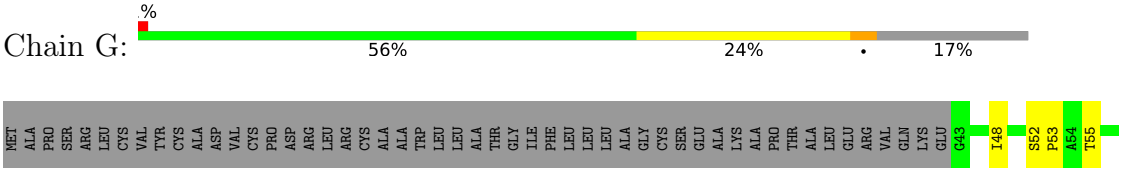
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

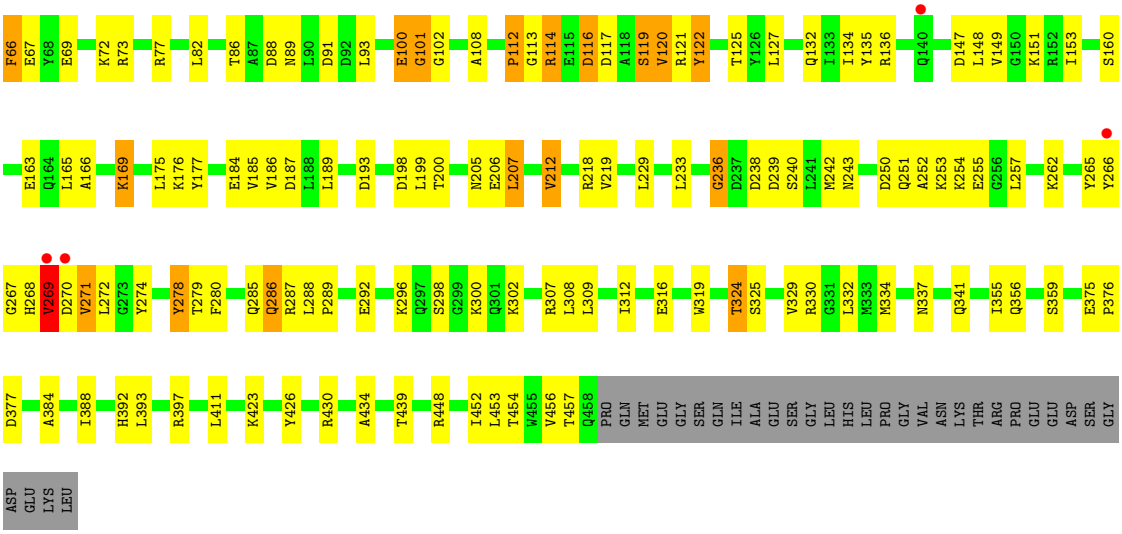
Chain F:



• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

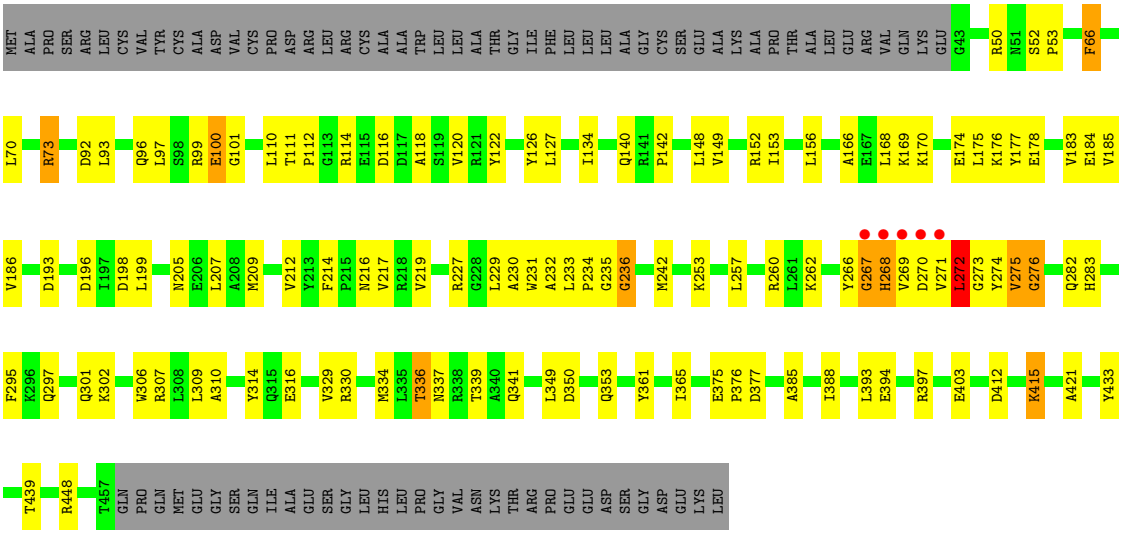
Chain G:





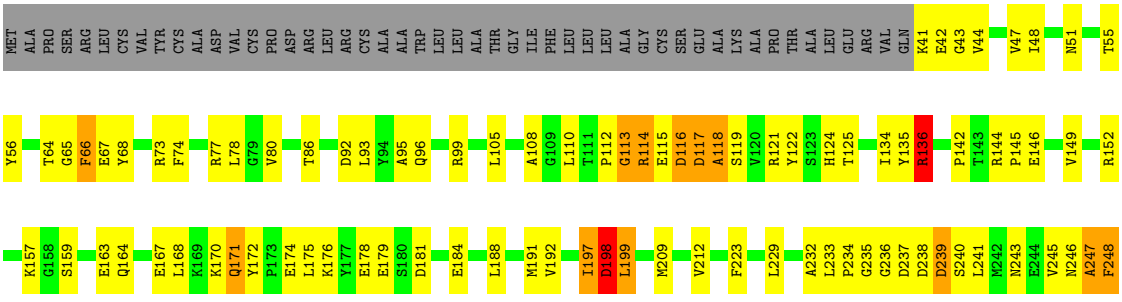
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

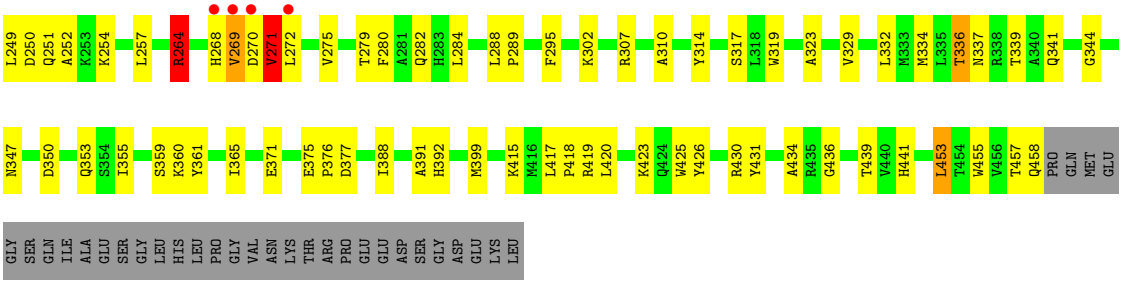
Chain H:



• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

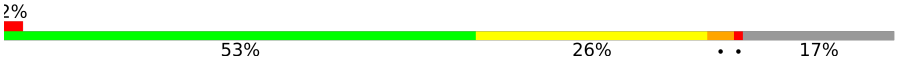
Chain I:

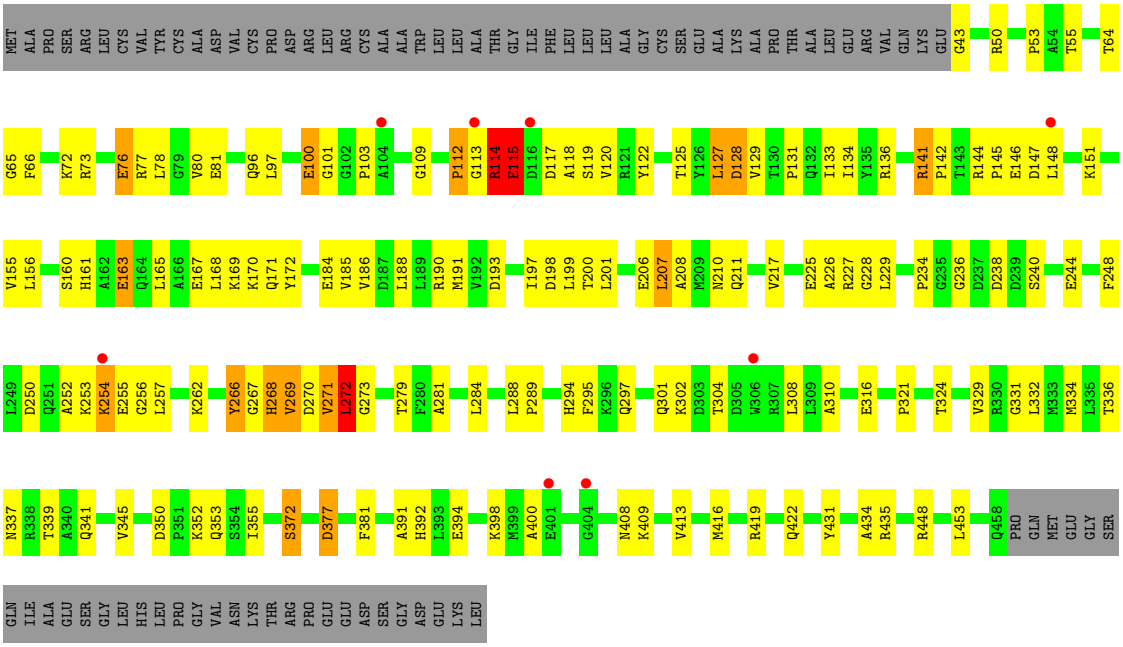




• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

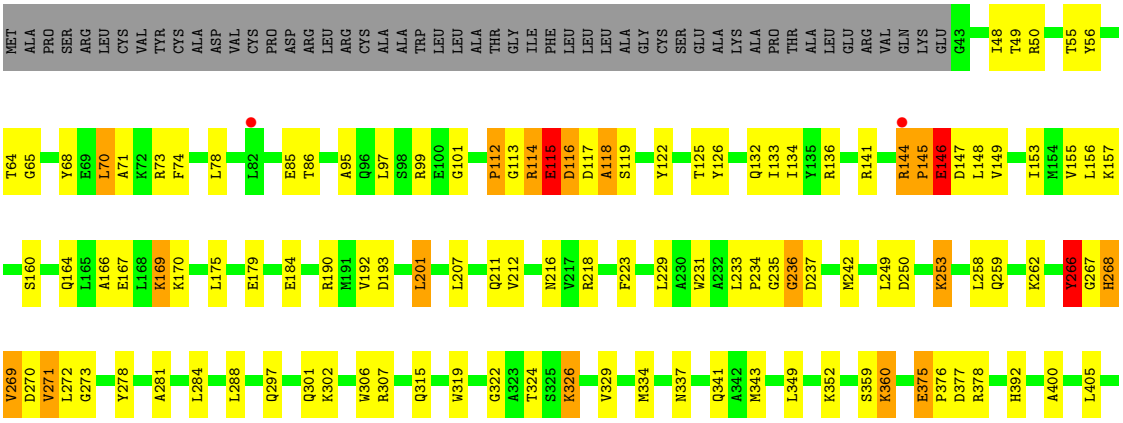
Chain J:

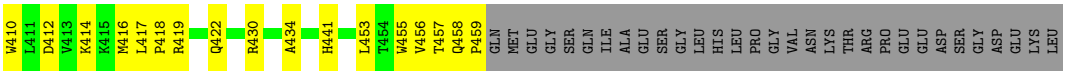




• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

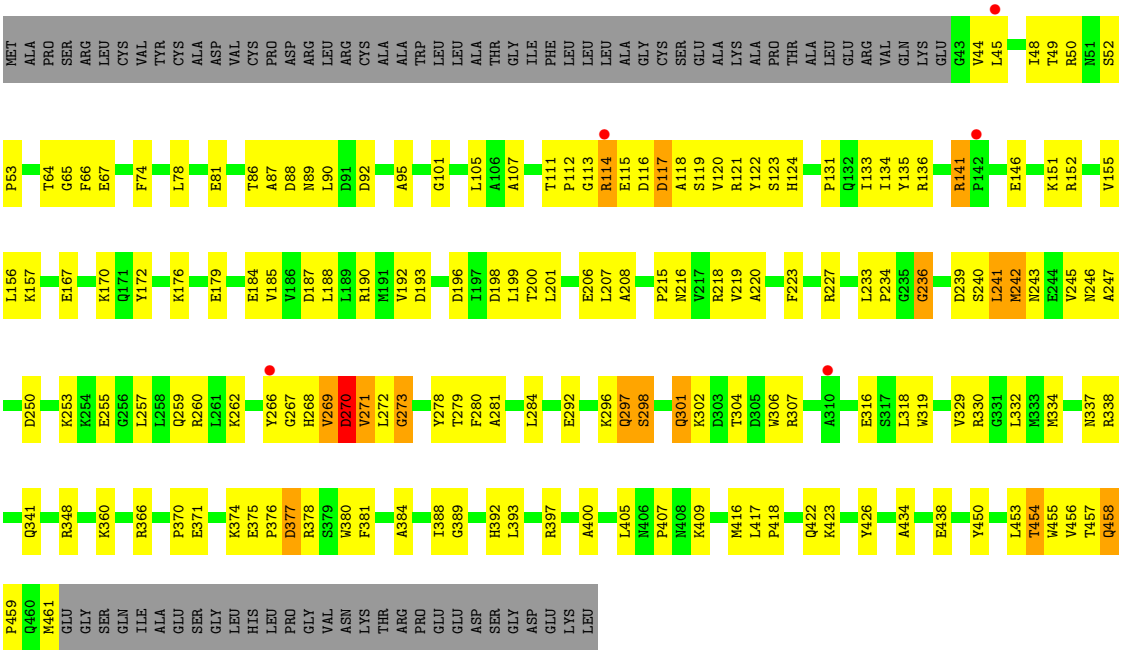
Chain K:





• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	150.60Å 136.38Å 195.39Å 90.00° 111.38° 90.00°	Depositor
Resolution (Å)	14.99 – 3.20 48.89 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (14.99-3.20) 99.1 (48.89-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.240 , 0.305 0.252 , 0.315	Depositor DCC
R_{free} test set	6091 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	74.1	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40234	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2751e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.68	0/3433	0.88	7/4642 (0.2%)
1	B	0.71	0/3421	0.88	2/4624 (0.0%)
1	C	0.73	1/3442 (0.0%)	0.87	3/4654 (0.1%)
1	D	0.68	0/3403	0.84	0/4600
1	E	0.65	0/3429	0.83	0/4636
1	F	0.65	0/3421	0.83	1/4624 (0.0%)
1	G	0.64	0/3412	0.77	1/4612 (0.0%)
1	H	0.64	0/3403	0.81	1/4600 (0.0%)
1	I	0.67	0/3430	0.88	5/4635 (0.1%)
1	J	0.55	0/3412	0.76	2/4612 (0.0%)
1	K	0.60	0/3420	0.82	2/4624 (0.0%)
1	L	0.56	0/3437	0.79	1/4646 (0.0%)
All	All	0.65	1/41063 (0.0%)	0.83	25/55509 (0.0%)

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	A	0	1
1	D	0	1
1	I	0	2
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	GLU	CB-CG	-5.01	1.42	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	198	ASP	N-CA-C	7.98	132.54	111.00
1	I	136	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	J	272	LEU	CA-CB-CG	6.66	130.61	115.30
1	C	448	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	330	ARG	NE-CZ-NH1	-6.45	117.08	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	VAL	Peptide
1	D	114	ARG	Peptide
1	I	115	GLU	Peptide
1	I	197	ILE	Peptide
1	J	254	LYS	Peptide

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	3361	0	3302	112	0
1	B	3351	0	3293	112	0
1	C	3370	0	3308	111	0
1	D	3333	0	3279	135	1
1	E	3358	0	3302	128	1
1	F	3351	0	3294	122	0
1	G	3342	0	3287	147	0
1	H	3333	0	3279	110	0
1	I	3360	0	3306	172	0
1	J	3342	0	3287	138	0
1	K	3349	0	3294	143	1
1	L	3366	0	3311	152	1
2	A	10	8	5	7	0
All	All	40226	8	39547	1560	2

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 20.

The worst 5 of 1560 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:117:ASP:O	1:A:119:SER:N	1.63	1.31
1:K:144:ARG:HG3	1:K:145:PRO:HD2	1.27	1.14
1:B:457:THR:HA	1:B:458:GLN:HB2	1.28	1.14
1:A:212:VAL:HG21	1:A:269:VAL:HG22	1.17	1.12
1:D:114:ARG:HB2	1:D:115:GLU:HG3	1.21	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:GLU:OE1	1:L:278:TYR:OH[1_545]	2.10	0.10
1:D:292:GLU:OE1	1:K:278:TYR:OH[1_655]	2.15	0.05

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	417/499 (84%)	389 (93%)	21 (5%)	7 (2%)	9 42
1	B	416/499 (83%)	398 (96%)	16 (4%)	2 (0%)	29 67
1	C	418/499 (84%)	396 (95%)	19 (4%)	3 (1%)	22 61
1	D	414/499 (83%)	392 (95%)	14 (3%)	8 (2%)	8 39
1	E	417/499 (84%)	395 (95%)	17 (4%)	5 (1%)	13 49
1	F	416/499 (83%)	391 (94%)	19 (5%)	6 (1%)	11 46
1	G	415/499 (83%)	393 (95%)	12 (3%)	10 (2%)	6 34
1	H	414/499 (83%)	393 (95%)	16 (4%)	5 (1%)	13 49
1	I	417/499 (84%)	387 (93%)	19 (5%)	11 (3%)	5 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	415/499 (83%)	387 (93%)	19 (5%)	9 (2%)	6 35
1	K	416/499 (83%)	383 (92%)	17 (4%)	16 (4%)	3 22
1	L	418/499 (84%)	385 (92%)	21 (5%)	12 (3%)	4 28
All	All	4993/5988 (83%)	4689 (94%)	210 (4%)	94 (2%)	8 39

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	GLY
1	A	115	GLU
1	A	118	ALA
1	A	271	VAL
1	B	118	ALA

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	349/413 (84%)	335 (96%)	14 (4%)	31 66
1	B	348/413 (84%)	335 (96%)	13 (4%)	34 68
1	C	350/413 (85%)	333 (95%)	17 (5%)	25 61
1	D	346/413 (84%)	331 (96%)	15 (4%)	29 64
1	E	349/413 (84%)	338 (97%)	11 (3%)	39 71
1	F	348/413 (84%)	336 (97%)	12 (3%)	37 70
1	G	347/413 (84%)	332 (96%)	15 (4%)	29 64
1	H	346/413 (84%)	337 (97%)	9 (3%)	46 76
1	I	349/413 (84%)	337 (97%)	12 (3%)	37 70
1	J	347/413 (84%)	331 (95%)	16 (5%)	27 63
1	K	348/413 (84%)	336 (97%)	12 (3%)	37 70
1	L	350/413 (85%)	338 (97%)	12 (3%)	37 70
All	All	4177/4956 (84%)	4019 (96%)	158 (4%)	34 67

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	377	ASP
1	K	360	LYS
1	J	100	GLU
1	J	279	THR
1	L	279	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	356	GLN
1	J	61	ASN
1	K	268	HIS
1	J	171	GLN
1	E	445	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	GLU	A	501	-	8,9,9	1.34	1 (12%)	10,11,11	0.98	0

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	GLU	A	501	-	-	4/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GLU	CG-CD	2.06	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GLU	O-C-CA-N
2	A	501	GLU	O-C-CA-CB
2	A	501	GLU	OXT-C-CA-N
2	A	501	GLU	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GLU	7	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

6.1 Protein, DNA and RNA chains

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^{th} 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	417/499 (83%)	-0.24	3 (0%)	87	81	42, 60, 97, 136	0
1	B	417/499 (83%)	-0.30	1 (0%)	95	94	37, 58, 92, 159	0
1	C	418/499 (83%)	-0.27	3 (0%)	87	81	34, 60, 92, 134	0
1	D	415/499 (83%)	-0.24	4 (0%)	82	72	40, 64, 99, 141	0
1	E	418/499 (83%)	-0.26	4 (0%)	82	72	42, 65, 97, 150	0
1	F	416/499 (83%)	-0.29	4 (0%)	82	72	45, 65, 96, 135	0
1	G	416/499 (83%)	-0.23	4 (0%)	82	72	42, 72, 107, 148	0
1	H	415/499 (83%)	-0.27	5 (1%)	79	67	36, 68, 104, 160	0
1	I	418/499 (83%)	-0.22	4 (0%)	82	72	39, 69, 105, 144	0
1	J	416/499 (83%)	-0.06	8 (1%)	66	53	62, 85, 118, 135	0
1	K	417/499 (83%)	-0.09	2 (0%)	91	86	55, 81, 118, 154	0
1	L	419/499 (83%)	-0.08	5 (1%)	79	67	54, 80, 120, 179	0
All	All	5002/5988 (83%)	-0.21	47 (0%)	84	75	34, 70, 108, 179	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	271	VAL	7.5
1	I	270	ASP	6.1
1	D	270	ASP	4.9
1	E	270	ASP	4.5
1	G	270	ASP	4.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	GLU	A	501	10/10	0.76	0.52	19,81,82,83	0

6.5 Other polymers (i)

There are no such residues in this entry.