



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 11:07 PM UTC

PDB ID : 5AA3 / pdb\_00005aa3  
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](mailto: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  
Mogul : 2022.3.0, CSD as543be (2022)  
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

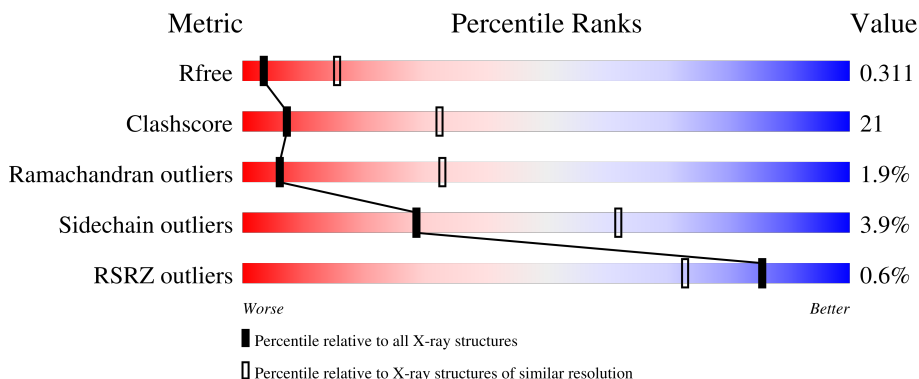
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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  $\geq 3$ , 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	499	 57% 24% 16%
1	B	499	 54% 27% 16%
1	C	499	 53% 28% 16%
1	D	499	 54% 25% 17%
1	E	499	 55% 26% 16%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain			
1	F	499				
1	G	499				
1	H	499				
1	I	499				
1	J	499				
1	K	499				
1	L	499				

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	-

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

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	VAL	-	expression tag	UNP Q9HYN1
C	5	CYS	-	expression tag	UNP Q9HYN1
C	6	PRO	-	expression tag	UNP Q9HYN1
C	7	ASP	-	expression tag	UNP Q9HYN1
C	302	LYS	LEU	conflict	UNP Q9HYN1
D	-8	MET	-	expression tag	UNP Q9HYN1
D	-7	ALA	-	expression tag	UNP Q9HYN1
D	-6	PRO	-	expression tag	UNP Q9HYN1
D	-5	SER	-	expression tag	UNP Q9HYN1
D	-4	ARG	-	expression tag	UNP Q9HYN1
D	-3	LEU	-	expression tag	UNP Q9HYN1
D	-2	CYS	-	expression tag	UNP Q9HYN1
D	-1	VAL	-	expression tag	UNP Q9HYN1
D	0	TYR	-	expression tag	UNP Q9HYN1
D	1	CYS	-	expression tag	UNP Q9HYN1
D	2	ALA	-	expression tag	UNP Q9HYN1
D	3	ASP	-	expression tag	UNP Q9HYN1
D	4	VAL	-	expression tag	UNP Q9HYN1
D	5	CYS	-	expression tag	UNP Q9HYN1
D	6	PRO	-	expression tag	UNP Q9HYN1
D	7	ASP	-	expression tag	UNP Q9HYN1
D	302	LYS	LEU	conflict	UNP Q9HYN1
E	-8	MET	-	expression tag	UNP Q9HYN1
E	-7	ALA	-	expression tag	UNP Q9HYN1
E	-6	PRO	-	expression tag	UNP Q9HYN1
E	-5	SER	-	expression tag	UNP Q9HYN1
E	-4	ARG	-	expression tag	UNP Q9HYN1
E	-3	LEU	-	expression tag	UNP Q9HYN1
E	-2	CYS	-	expression tag	UNP Q9HYN1
E	-1	VAL	-	expression tag	UNP Q9HYN1
E	0	TYR	-	expression tag	UNP Q9HYN1
E	1	CYS	-	expression tag	UNP Q9HYN1
E	2	ALA	-	expression tag	UNP Q9HYN1
E	3	ASP	-	expression tag	UNP Q9HYN1
E	4	VAL	-	expression tag	UNP Q9HYN1
E	5	CYS	-	expression tag	UNP Q9HYN1
E	6	PRO	-	expression tag	UNP Q9HYN1
E	7	ASP	-	expression tag	UNP Q9HYN1
E	302	LYS	LEU	conflict	UNP Q9HYN1
F	-8	MET	-	expression tag	UNP Q9HYN1
F	-7	ALA	-	expression tag	UNP Q9HYN1
F	-6	PRO	-	expression tag	UNP Q9HYN1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	SER	-	expression tag	UNP Q9HYN1
F	-4	ARG	-	expression tag	UNP Q9HYN1
F	-3	LEU	-	expression tag	UNP Q9HYN1
F	-2	CYS	-	expression tag	UNP Q9HYN1
F	-1	VAL	-	expression tag	UNP Q9HYN1
F	0	TYR	-	expression tag	UNP Q9HYN1
F	1	CYS	-	expression tag	UNP Q9HYN1
F	2	ALA	-	expression tag	UNP Q9HYN1
F	3	ASP	-	expression tag	UNP Q9HYN1
F	4	VAL	-	expression tag	UNP Q9HYN1
F	5	CYS	-	expression tag	UNP Q9HYN1
F	6	PRO	-	expression tag	UNP Q9HYN1
F	7	ASP	-	expression tag	UNP Q9HYN1
F	302	LYS	LEU	conflict	UNP Q9HYN1
G	-8	MET	-	expression tag	UNP Q9HYN1
G	-7	ALA	-	expression tag	UNP Q9HYN1
G	-6	PRO	-	expression tag	UNP Q9HYN1
G	-5	SER	-	expression tag	UNP Q9HYN1
G	-4	ARG	-	expression tag	UNP Q9HYN1
G	-3	LEU	-	expression tag	UNP Q9HYN1
G	-2	CYS	-	expression tag	UNP Q9HYN1
G	-1	VAL	-	expression tag	UNP Q9HYN1
G	0	TYR	-	expression tag	UNP Q9HYN1
G	1	CYS	-	expression tag	UNP Q9HYN1
G	2	ALA	-	expression tag	UNP Q9HYN1
G	3	ASP	-	expression tag	UNP Q9HYN1
G	4	VAL	-	expression tag	UNP Q9HYN1
G	5	CYS	-	expression tag	UNP Q9HYN1
G	6	PRO	-	expression tag	UNP Q9HYN1
G	7	ASP	-	expression tag	UNP Q9HYN1
G	302	LYS	LEU	conflict	UNP Q9HYN1
H	-8	MET	-	expression tag	UNP Q9HYN1
H	-7	ALA	-	expression tag	UNP Q9HYN1
H	-6	PRO	-	expression tag	UNP Q9HYN1
H	-5	SER	-	expression tag	UNP Q9HYN1
H	-4	ARG	-	expression tag	UNP Q9HYN1
H	-3	LEU	-	expression tag	UNP Q9HYN1
H	-2	CYS	-	expression tag	UNP Q9HYN1
H	-1	VAL	-	expression tag	UNP Q9HYN1
H	0	TYR	-	expression tag	UNP Q9HYN1
H	1	CYS	-	expression tag	UNP Q9HYN1
H	2	ALA	-	expression tag	UNP Q9HYN1

*Continued on next page...*

*Continued from previous page...*

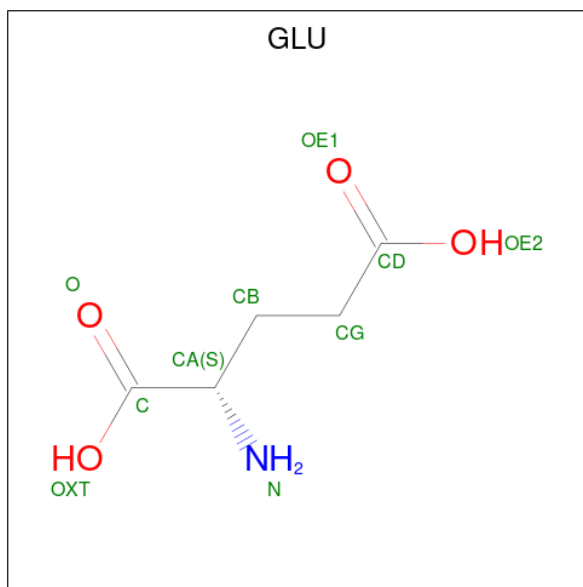
Chain	Residue	Modelled	Actual	Comment	Reference
H	3	ASP	-	expression tag	UNP Q9HXN1
H	4	VAL	-	expression tag	UNP Q9HXN1
H	5	CYS	-	expression tag	UNP Q9HXN1
H	6	PRO	-	expression tag	UNP Q9HXN1
H	7	ASP	-	expression tag	UNP Q9HXN1
H	302	LYS	LEU	conflict	UNP Q9HXN1
I	-8	MET	-	expression tag	UNP Q9HXN1
I	-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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	PRO	-	expression tag	UNP Q9HYN1
K	-5	SER	-	expression tag	UNP Q9HYN1
K	-4	ARG	-	expression tag	UNP Q9HYN1
K	-3	LEU	-	expression tag	UNP Q9HYN1
K	-2	CYS	-	expression tag	UNP Q9HYN1
K	-1	VAL	-	expression tag	UNP Q9HYN1
K	0	TYR	-	expression tag	UNP Q9HYN1
K	1	CYS	-	expression tag	UNP Q9HYN1
K	2	ALA	-	expression tag	UNP Q9HYN1
K	3	ASP	-	expression tag	UNP Q9HYN1
K	4	VAL	-	expression tag	UNP Q9HYN1
K	5	CYS	-	expression tag	UNP Q9HYN1
K	6	PRO	-	expression tag	UNP Q9HYN1
K	7	ASP	-	expression tag	UNP Q9HYN1
K	302	LYS	LEU	conflict	UNP Q9HYN1
L	-8	MET	-	expression tag	UNP Q9HYN1
L	-7	ALA	-	expression tag	UNP Q9HYN1
L	-6	PRO	-	expression tag	UNP Q9HYN1
L	-5	SER	-	expression tag	UNP Q9HYN1
L	-4	ARG	-	expression tag	UNP Q9HYN1
L	-3	LEU	-	expression tag	UNP Q9HYN1
L	-2	CYS	-	expression tag	UNP Q9HYN1
L	-1	VAL	-	expression tag	UNP Q9HYN1
L	0	TYR	-	expression tag	UNP Q9HYN1
L	1	CYS	-	expression tag	UNP Q9HYN1
L	2	ALA	-	expression tag	UNP Q9HYN1
L	3	ASP	-	expression tag	UNP Q9HYN1
L	4	VAL	-	expression tag	UNP Q9HYN1
L	5	CYS	-	expression tag	UNP Q9HYN1
L	6	PRO	-	expression tag	UNP Q9HYN1
L	7	ASP	-	expression tag	UNP Q9HYN1
L	302	LYS	LEU	conflict	UNP Q9HYN1

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).

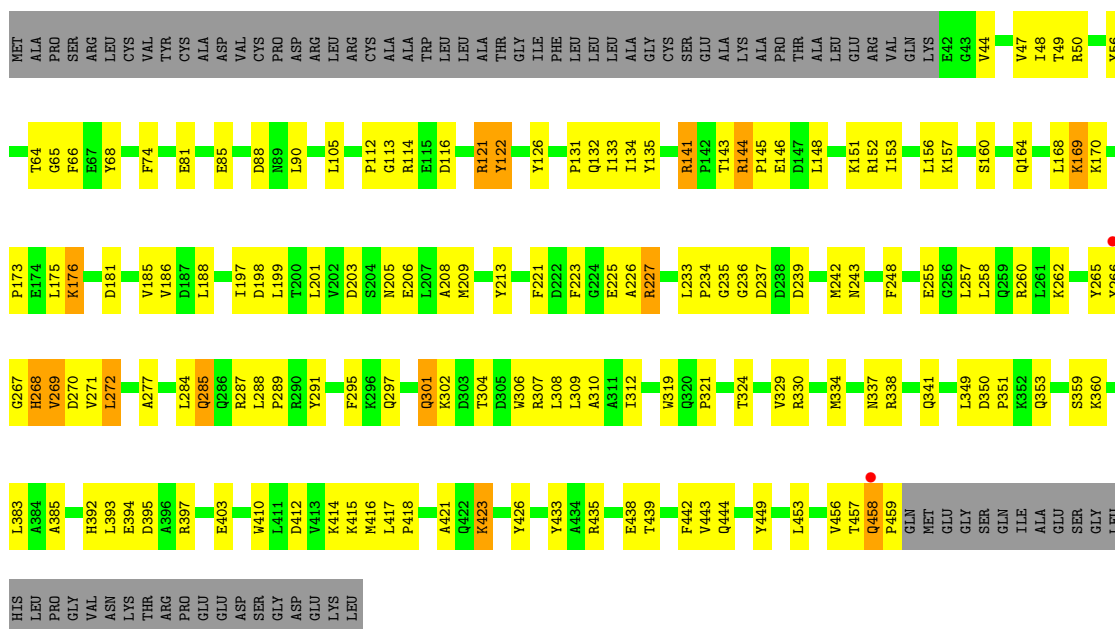


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	18	5	8	1	4	0	0

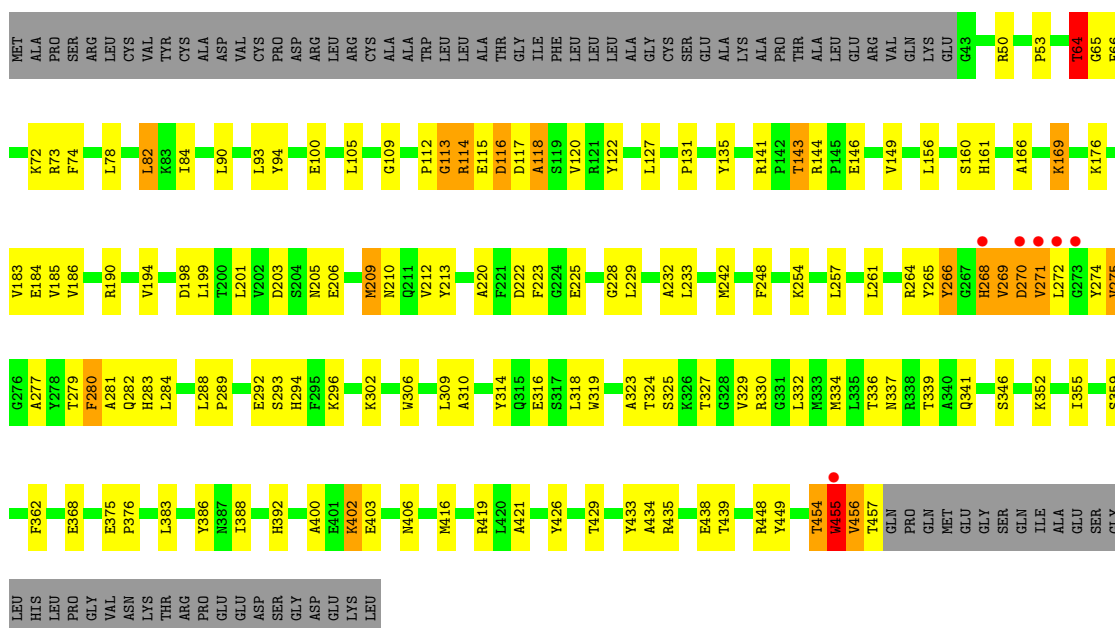




● Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

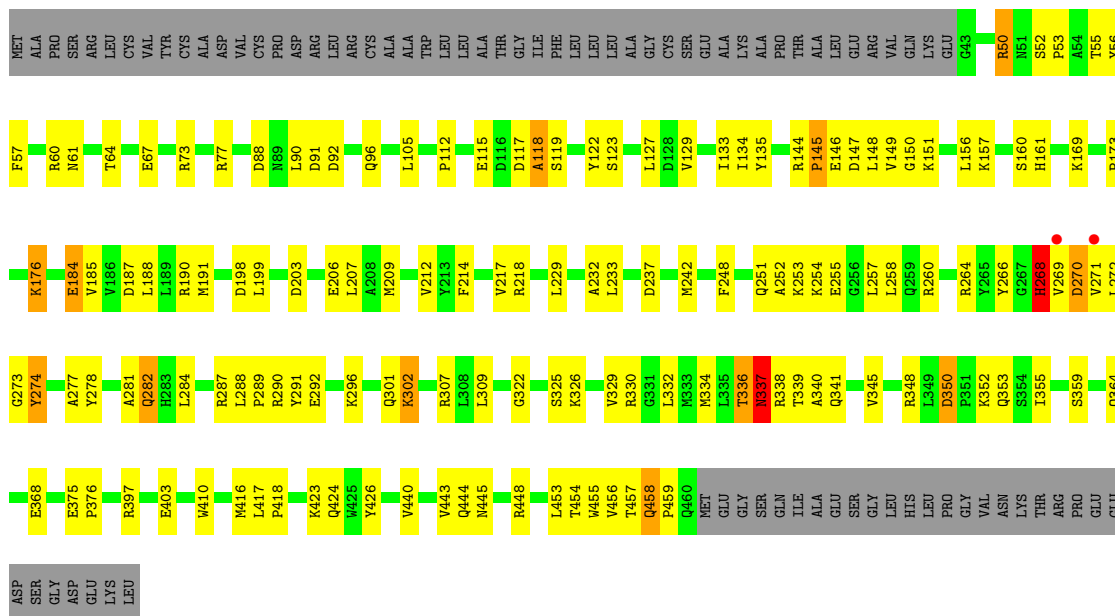


● Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



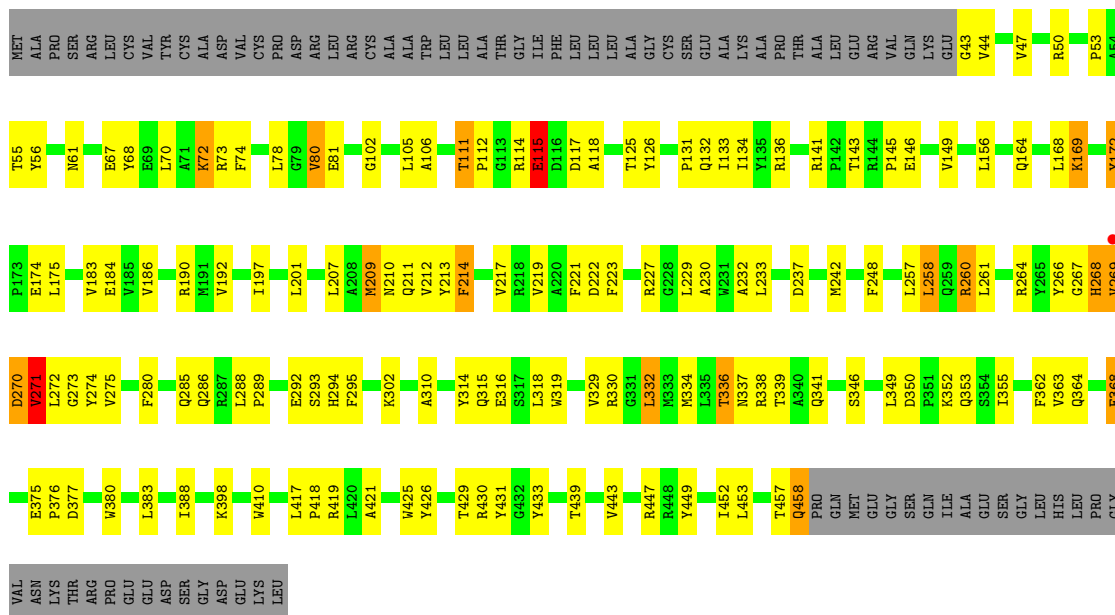
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain E:  55% 26% 16%



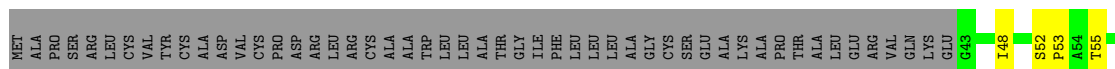
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

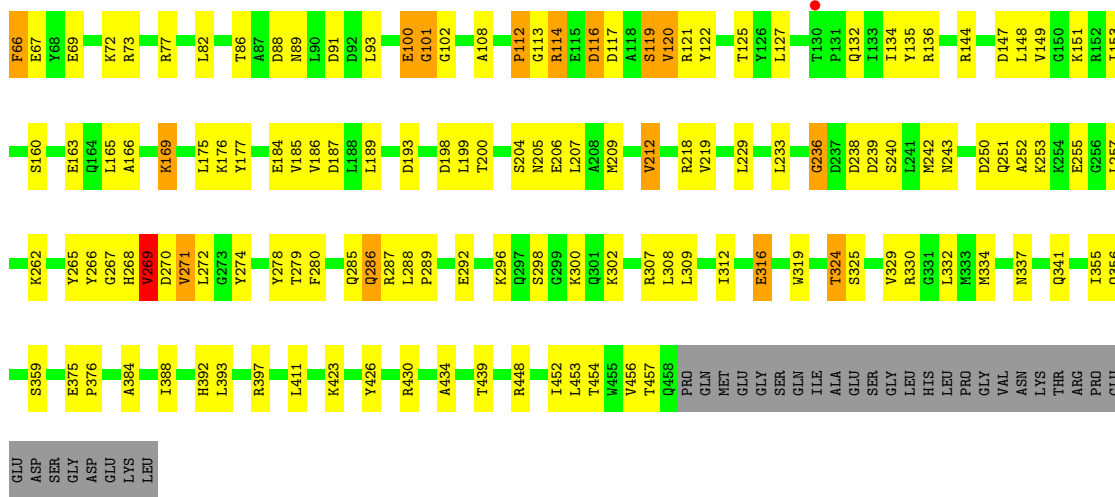
Chain F:  54% 26% 17%



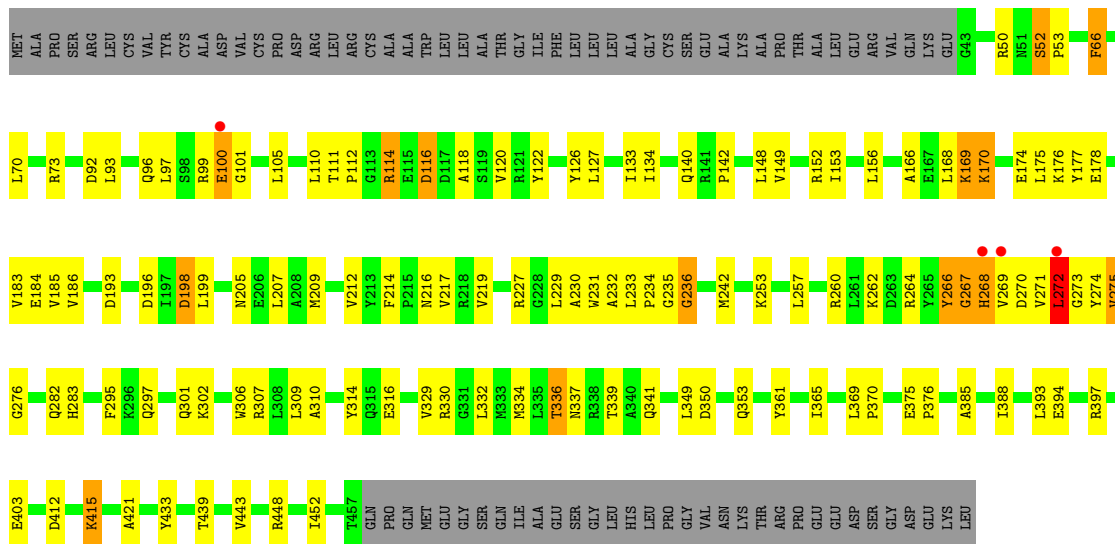
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain G:  56% 25% 17%

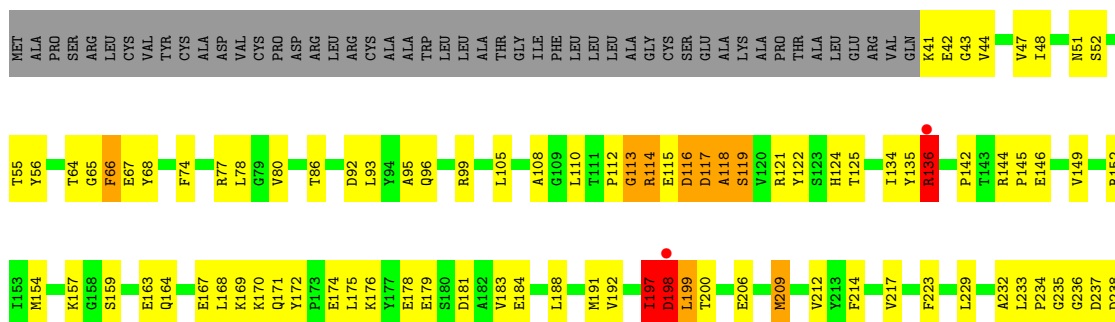




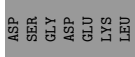
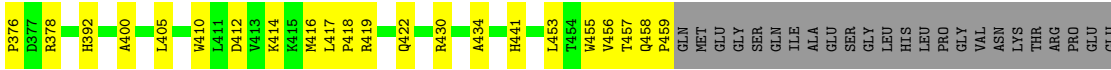
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



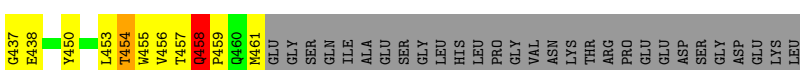
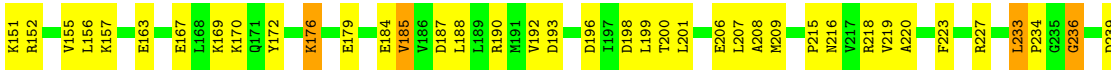
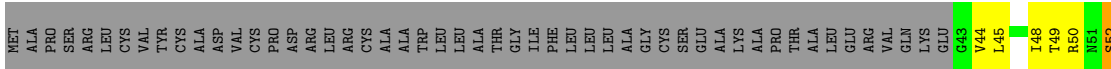
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F







● Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.60Å 136.38Å 195.39Å 90.00° 111.38° 90.00°	Depositor
Resolution (Å)	14.99 – 3.20 14.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (14.99-3.20) 98.1 (14.99-3.20)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.240 , 0.305 0.252 , 0.311	Depositor DCC
$R_{free}$ test set	6091 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.1	Xtrriage
Anisotropy	0.103	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	40234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage'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.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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	0.86	1/3433 (0.0%)	1.18	10/4642 (0.2%)
1	B	0.88	2/3421 (0.1%)	1.22	17/4624 (0.4%)
1	C	0.91	1/3442 (0.0%)	1.16	12/4654 (0.3%)
1	D	0.85	0/3403	1.17	10/4600 (0.2%)
1	E	0.83	0/3429	1.17	14/4636 (0.3%)
1	F	0.79	0/3421	1.13	10/4624 (0.2%)
1	G	0.79	0/3412	1.07	4/4612 (0.1%)
1	H	0.81	1/3403 (0.0%)	1.15	6/4600 (0.1%)
1	I	0.84	0/3430	1.17	12/4635 (0.3%)
1	J	0.71	1/3412 (0.0%)	1.09	6/4612 (0.1%)
1	K	0.75	0/3420	1.12	13/4624 (0.3%)
1	L	0.73	0/3437	1.11	11/4646 (0.2%)
All	All	0.81	6/41063 (0.0%)	1.15	125/55509 (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	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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	116	ASP	CA-C	6.65	1.55	1.52
1	A	322	GLY	C-O	-5.78	1.18	1.24

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	443	VAL	CA-CB	-5.26	1.48	1.54
1	B	446	VAL	CA-C	-5.20	1.46	1.52
1	C	385	ALA	CA-CB	-5.18	1.45	1.53

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	148	LEU	N-CA-C	-11.31	99.51	113.20
1	H	114	ARG	N-CA-C	10.38	124.06	111.40
1	I	198	ASP	N-CA-C	10.21	132.54	110.80
1	K	277	ALA	N-CA-C	-9.04	101.33	111.82
1	A	277	ALA	N-CA-C	-8.82	101.58	111.82

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

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	121	0
1	B	3351	0	3293	117	0
1	C	3370	0	3308	119	0
1	D	3333	0	3279	136	1
1	E	3358	0	3302	134	1
1	F	3351	0	3294	130	0
1	G	3342	0	3287	149	0
1	H	3333	0	3279	117	0
1	I	3360	0	3306	180	0
1	J	3342	0	3287	145	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3349	0	3294	151	1
1	L	3366	0	3311	165	1
2	A	10	8	5	7	0
All	All	40226	8	39547	1640	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 21.

The worst 5 of 1640 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%)	7	35
1	B	416/499 (83%)	398 (96%)	16 (4%)	2 (0%)	24	59

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	418/499 (84%)	396 (95%)	19 (4%)	3 (1%)	18	52
1	D	414/499 (83%)	392 (95%)	14 (3%)	8 (2%)	6	33
1	E	417/499 (84%)	395 (95%)	17 (4%)	5 (1%)	10	42
1	F	416/499 (83%)	391 (94%)	19 (5%)	6 (1%)	9	39
1	G	415/499 (83%)	393 (95%)	12 (3%)	10 (2%)	4	28
1	H	414/499 (83%)	393 (95%)	16 (4%)	5 (1%)	10	42
1	I	417/499 (84%)	387 (93%)	19 (5%)	11 (3%)	4	26
1	J	415/499 (83%)	387 (93%)	19 (5%)	9 (2%)	5	29
1	K	416/499 (83%)	383 (92%)	17 (4%)	16 (4%)	2	18
1	L	418/499 (84%)	385 (92%)	21 (5%)	12 (3%)	3	24
All	All	4993/5988 (83%)	4689 (94%)	210 (4%)	94 (2%)	6	33

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%)	334 (96%)	15 (4%)	26	59
1	B	348/413 (84%)	335 (96%)	13 (4%)	30	63
1	C	350/413 (85%)	334 (95%)	16 (5%)	24	58
1	D	346/413 (84%)	331 (96%)	15 (4%)	26	59
1	E	349/413 (84%)	335 (96%)	14 (4%)	28	61
1	F	348/413 (84%)	334 (96%)	14 (4%)	28	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	347/413 (84%)	335 (96%)	12 (4%)	32	64
1	H	346/413 (84%)	335 (97%)	11 (3%)	34	65
1	I	349/413 (84%)	338 (97%)	11 (3%)	34	65
1	J	347/413 (84%)	332 (96%)	15 (4%)	26	59
1	K	348/413 (84%)	337 (97%)	11 (3%)	34	65
1	L	350/413 (85%)	335 (96%)	15 (4%)	26	59
All	All	4177/4956 (84%)	4015 (96%)	162 (4%)	28	62

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	217	VAL
1	K	217	VAL
1	I	336	THR
1	J	266	TYR
1	L	169	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	132	GLN
1	I	243	ASN
1	K	387	ASN
1	H	164	GLN
1	H	337	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 oligosaccharides 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	1.37	1 (12%)	8,11,11	1.04	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	2.07	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	OXT-C-CA-N
2	A	501	GLU	O-C-CA-CB
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 [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	417/499 (83%)	-0.45	4 (0%) 79 63	23, 60, 97, 136	2 (0%)
1	B	417/499 (83%)	-0.50	0 100 100	22, 58, 92, 159	1 (0%)
1	C	418/499 (83%)	-0.43	2 (0%) 87 76	23, 60, 92, 134	2 (0%)
1	D	415/499 (83%)	-0.43	6 (1%) 73 54	28, 64, 99, 141	1 (0%)
1	E	418/499 (83%)	-0.45	2 (0%) 87 76	28, 65, 97, 150	1 (0%)
1	F	416/499 (83%)	-0.51	1 (0%) 91 85	31, 65, 96, 135	2 (0%)
1	G	416/499 (83%)	-0.40	1 (0%) 91 85	32, 72, 107, 148	1 (0%)
1	H	415/499 (83%)	-0.39	4 (0%) 79 63	28, 68, 104, 160	1 (0%)
1	I	418/499 (83%)	-0.35	4 (0%) 79 63	28, 69, 105, 144	1 (0%)
1	J	416/499 (83%)	-0.25	1 (0%) 91 85	34, 85, 118, 135	1 (0%)
1	K	417/499 (83%)	-0.26	2 (0%) 87 76	31, 81, 118, 154	1 (0%)
1	L	419/499 (83%)	-0.24	1 (0%) 91 85	31, 80, 120, 179	1 (0%)
All	All	5002/5988 (83%)	-0.39	28 (0%) 85 73	22, 70, 108, 179	15 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	266	TYR	3.8
1	A	117	ASP	3.4
1	A	272	LEU	3.4
1	E	271	VAL	3.3
1	C	266[A]	TYR	3.2

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLU	A	501	10/10	0.70	0.21	19,81,82,83	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.