

Full wwPDB X-ray Structure Validation Report (i)

Dec 20, 2023 – 01:22 pm GMT

PDB ID	:	8BZ4
Title	:	Crystal structure of the apo form of the L. monocytogenes RmlT
Authors	:	Cereija, T.B.; Morais-Cabral, J.H.
Deposited on	:	2022-12-14
Resolution	:	2.52 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.52 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.



Motrie	Whole archive	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	130704	5743 (2.54-2.50)		
Clashscore	141614	6463 (2.54-2.50)		
Ramachandran outliers	138981	6335 (2.54-2.50)		
Sidechain outliers	138945	6337 (2.54-2.50)		
RSRZ outliers	127900	5630(2.54-2.50)		

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	А	624	89%		8% •
1	В	624	77%	15%	8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9848 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	606	Total 4915	C 3132	N 817	0 954	S 1	Se 11	0	1	0
1	В	577	Total 4691	C 2999	N 780	O 900	S 1	Se 11	16	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	GLY	-	expression tag	UNP A0A401AAP7
В	0	GLY	-	expression tag	UNP A0A401AAP7

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Cl 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	206	Total O 206 206	0	0
3	В	35	Total O 35 35	0	0



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: Glycosyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	83.43Å 103.69Å 178.41Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$Resolution(\AA)$	49.78 - 2.52	Depositor
Resolution (A)	49.78 - 2.52	EDS
% Data completeness	$100.0 \ (49.78-2.52)$	Depositor
(in resolution range)	$100.0 \ (49.78-2.52)$	EDS
R _{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) > 1$	$1.67 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
P. P.	0.219 , 0.251	Depositor
n, n_{free}	0.219 , 0.253	DCC
R_{free} test set	2572 reflections $(4.85%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	51.6	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31,43.4	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9848	wwPDB-VP
Average B, all atoms $(Å^2)$	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: CL

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	А	0.26	0/5005	0.47	0/6741	
1	В	0.26	0/4774	0.47	0/6423	
All	All	0.26	0/9779	0.47	0/13164	

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	А	4915	0	4849	28	0
1	В	4691	0	4647	57	0
2	А	1	0	0	0	0
3	А	206	0	0	2	0
3	В	35	0	0	0	0
All	All	9848	0	9496	85	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 4.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:595:LEU:HD12	1:B:595:LEU:O	1.66	0.96
1:A:146:SER:HA	1:A:423:THR:HG21	1.65	0.76
1:A:267:THR:HG22	1:A:309:ILE:HG23	1.69	0.73
1:B:431:SER:HB3	1:B:449:MSE:HG3	1.69	0.73
1:B:415:ILE:HB	1:B:426:ILE:HD11	1.72	0.71
1:B:595:LEU:HD13	1:B:598:GLU:HB3	1.76	0.68
1:B:595:LEU:O	1:B:595:LEU:CD1	2.43	0.66
1:A:413:PRO:HG2	1:A:426:ILE:HB	1.76	0.66
1:A:531:LYS:HB3	1:A:534:GLN:HB2	1.76	0.66
1:B:22:SER:HB2	1:B:106:ILE:HG22	1.79	0.65
1:B:413:PRO:HG2	1:B:426:ILE:HB	1.79	0.64
1:A:383:MSE:HG3	1:A:406:LEU:HD11	1.79	0.62
1:B:197:GLU:HA	1:B:200:TYR:HD2	1.64	0.62
1:B:582:LEU:HD23	1:B:591:VAL:HG22	1.83	0.60
1:B:35:LEU:HD23	1:B:35:LEU:H	1.67	0.59
1:B:544:VAL:HB	1:B:593:VAL:HB	1.86	0.58
1:A:370:ASP:OD1	1:A:484:ARG:NH2	2.37	0.57
1:A:570:ILE:HB	1:A:573:ALA:HB2	1.87	0.57
1:B:508:ASN:HD21	1:B:512:LEU:HB2	1.69	0.56
1:B:383:MSE:HG3	1:B:406:LEU:HD11	1.87	0.56
1:B:42:ILE:HD11	1:B:120:PHE:HZ	1.73	0.54
1:B:495:THR:HG22	1:B:504:ILE:HG12	1.90	0.54
1:B:429:SER:HB2	1:B:449:MSE:HE3	1.89	0.53
1:B:186:ILE:HD13	1:B:205:ALA:HA	1.91	0.53
1:A:64:ASP:OD1	1:A:64:ASP:N	2.38	0.52
1:B:138:LYS:HA	1:B:152:PHE:CD1	2.44	0.52
1:A:439:LYS:HE2	1:A:442:LEU:HD12	1.92	0.51
1:B:138:LYS:HB3	1:B:219:PRO:HA	1.92	0.51
1:B:168:LEU:HD23	1:B:170:MSE:HG3	1.92	0.51
1:B:134:VAL:O	1:B:212:VAL:HA	2.11	0.51
1:B:523:SER:HB2	1:B:613:LYS:HB3	1.93	0.50
1:A:492:LEU:O	1:A:506:TYR:HA	2.11	0.50
1:B:27:THR:HG23	1:B:30:THR:HB	1.91	0.50
1:A:159:ALA:O	1:A:162:MSE:HG2	2.11	0.50
1:A:377:GLU:HG3	1:A:386:ILE:HG12	1.94	0.49
1:B:558:LEU:HD21	1:B:581:LYS:HD2	1.94	0.49
1:B:537:ILE:HG21	1:B:623:LEU:HD11	1.94	0.49
1:B:492:LEU:O	1:B:506:TYR:HA	2.13	0.49
1:B:387:LEU:HB2	1:B:392:LYS:HG3	1.95	0.48
1:B:581:LYS:HE3	1:B:583:ILE:HD11	1.96	0.48
1:A:384:GLU:HG2	1:A:400:PHE:HD2	1.79	0.48
1:B:242:TRP:HE1	1:B:293:GLU:CG	2.27	0.48



	Interatomic Clash							
Atom-1	Atom-2	distance (Å)	overlap (Å)					
1:A:123:VAL:HG13	1:A:135:VAL:HG11	1.97	0.47					
1:A:132:LEU:HD13	1:A:213:GLY:HA3	1.96	0.47					
1:A:145:TRP:CZ2	1:A:485:ALA:HB2	2.50	0.47					
1:B:49:PRO:HA	1:B:52:TYR:CE1	2.49	0.47					
1:B:45:GLN:HG3	1:B:120:PHE:CE2	2.50	0.47					
1:B:603:GLU:HA	1:B:622:THR:HA	1.97	0.47					
1:B:138:LYS:HA	1:B:152:PHE:HD1	1.81	0.46					
1:B:546:ILE:HD11	1:B:606:LEU:HD13	1.97	0.46					
1:B:173:HIS:HB3	1:B:221:TYR:CG	2.50	0.46					
1:B:42:ILE:HD11	1:B:120:PHE:CZ	2.51	0.46					
1:B:354:LYS:HB3	1:B:359:PHE:CE1	2.51	0.45					
1:A:418:ARG:HB3	1:A:468:PRO:HG2	1.98	0.45					
1:B:410:THR:OG1	1:B:476:THR:HB	2.16	0.45					
1:B:145:TRP:CZ2	1:B:485:ALA:HB2	2.52	0.44					
1:B:137:GLY:HA2	1:B:215:LEU:HB3	1.99	0.44					
1:B:449:MSE:HE2	1:B:451:PHE:CD1	2.51	0.44					
1:A:378:LYS:HB2	1:A:383:MSE:SE	2.68	0.44					
1:B:139:GLU:HG3	1:B:221:TYR:HB3	2.00	0.44					
1:B:600:LEU:HD12	1:B:604:TYR:CZ	2.53	0.44					
1:A:186:ILE:HD13	1:A:205:ALA:HA	2.00	0.43					
1:B:356:ASP:HA	1:B:498:ILE:HD13	2.00	0.43					
1:A:260:ARG:NH2	3:A:816:HOH:O	2.50	0.43					
1:A:38:LEU:HD13	1:A:111:HIS:HA	2.00	0.43					
1:A:169:PRO:HG2	3:A:827:HOH:O	2.18	0.43					
1:A:565:LEU:HD11	1:A:595:LEU:HD21	2.01	0.43					
1:A:64:ASP:CG	1:A:68:ARG:HH22	2.22	0.42					
1:B:173:HIS:HB3	1:B:221:TYR:CD1	2.54	0.42					
1:B:455:ILE:HD11	1:B:469:TRP:CE2	2.54	0.42					
1:B:469:TRP:HB2	1:B:515:LEU:HB3	2.02	0.42					
1:B:270:TYR:CD1	1:B:305:ILE:HG13	2.55	0.42					
1:B:621:ILE:HD12	1:B:621:ILE:HA	1.93	0.42					
1:B:241:LYS:O	1:B:245:ILE:HG13	2.20	0.41					
1:B:498:ILE:HG12	1:B:554:PHE:HB3	2.02	0.41					
1:A:593:VAL:HG21	1:A:606:LEU:HD21	2.00	0.41					
1:B:54:LEU:HD12	1:B:79:MSE:HG3	2.01	0.41					
1:B:139:GLU:HB3	1:B:147:TRP:CD1	2.55	0.41					
1:B:39:MSE:HA	1:B:42:ILE:HG22	2.02	0.41					
1:B:413:PRO:HB3	1:B:449:MSE:HE1	2.02	0.41					
1:A:127:GLY:HA2	1:A:132:LEU:HD12	2.03	0.41					
1:B:142:THR:HA	1:B:421:ARG:HG2	2.03	0.40					
1:A:241:LYS:O	1:A:245:ILE:HG13	2.22	0.40					

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:B:565:LEU:HA	1:B:605:HIS:O	2.21	0.40	
1:A:567:PRO:HD2	1:A:573:ALA:HB1	2.03	0.40	

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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	Perce	ntiles
1	А	605/624~(97%)	585~(97%)	20 (3%)	0	100	100
1	В	567/624~(91%)	531 (94%)	36 (6%)	0	100	100
All	All	1172/1248~(94%)	1116 (95%)	56 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	Perce	$\mathbf{ntil}\epsilon$	s
1	А	538/541~(99%)	535~(99%)	3 (1%)	86	94	
1	В	513/541~(95%)	507~(99%)	6 (1%)	71	87	
All	All	1051/1082~(97%)	1042 (99%)	9 (1%)	78	91	

All (9) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	247	LYS
1	А	273	ARG
1	А	590	ARG
1	В	58	ASP
1	В	69	LEU
1	В	189	ASP
1	В	382	ARG
1	В	490	LYS
1	В	497	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	595/624~(95%)	0.04	3 (0%) 91 92	34, 49, 85, 149	0
1	В	566/624~(90%)	1.00	104 (18%) 1 1	50, 90, 151, 193	3~(0%)
All	All	1161/1248 (93%)	0.51	107 (9%) 9 9	34, 65, 139, 193	3 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res Type		RSRZ
1	В	571	SER	10.2
1	В	569	GLY	9.9
1	В	69	LEU	9.8
1	В	56	PHE	8.0
1	В	181	LEU	7.9
1	В	91	SER	7.0
1	В	81	VAL	6.8
1	В	68	ARG	6.3
1	В	536	LEU	5.9
1	В	570	ILE	5.9
1	В	537	ILE	5.6
1	В	101	ALA	5.4
1	В	593	VAL	5.4
1	В	594	LEU	5.3
1	В	99	LYS	5.0
1	В	182	LEU	5.0
1	В	595	LEU	4.9
1	В	598	GLU	4.6
1	В	29	ASN	4.5
1	В	93	PRO	4.5
1	В	50	ASP	4.4
1	В	66	TYR	4.4
1	В	559	ILE	4.4
1	В	106	ILE	4.4



8BZ4

Mol	Chain	Res	Type	RSRZ
1	В	558	LEU	4.4
1	В	575	PRO	4.2
1	В	600	LEU	4.2
1	В	23	VAL	4.1
1	В	597	ASP	4.1
1	В	123	VAL	4.0
1	В	572	ASP	4.0
1	В	623	LEU	3.9
1	В	543	LYS	3.8
1	В	25	VAL	3.7
1	В	601	SER	3.7
1	В	21	ILE	3.7
1	В	554	PHE	3.7
1	В	54	LEU	3.7
1	В	596	GLY	3.7
1	В	542	GLY	3.6
1	В	72	PHE	3.6
1	В	399	PHE	3.5
1	В	176	TYR	3.5
1	В	576	ILE	3.5
1	В	604	TYR	3.4
1	В	96	ILE	3.4
1	В	75	THR	3.4
1	В	578	VAL	3.3
1	В	42	ILE	3.3
1	В	28	TYR	3.2
1	В	94	ARG	3.1
1	В	497	LEU	3.1
1	В	157	PRO	3.1
1	В	134	VAL	3.1
1	В	120	PHE	2.9
1	В	76	ARG	2.9
1	В	40	ALA	2.9
1	В	205	ALA	2.9
1	В	183	GLU	2.8
1	В	201	PHE	2.8
1	В	465	LYS	2.8
1	В	622	THR	2.8
1	В	55	VAL	2.8
1	В	579	LYS	2.8
1	В	568	VAL	2.8
1	В	132	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	В	538	ASP	2.7
1	В	166	CYS	2.7
1	В	107	LEU	2.6
1	В	57	VAL	2.6
1	А	231	SER	2.6
1	В	541	SER	2.6
1	В	80	THR	2.6
1	В	175	PHE	2.6
1	В	179	GLU	2.6
1	В	49	PRO	2.5
1	В	581	LYS	2.5
1	В	498	ILE	2.5
1	В	187	THR	2.5
1	В	184	ASN	2.5
1	В	544	VAL	2.4
1	В	193	ARG	2.4
1	В	77	PRO	2.4
1	В	48	ASN	2.3
1	В	26	PRO	2.3
1	В	545	THR	2.3
1	В	402	TYR	2.3
1	В	574	ASP	2.2
1	В	186	ILE	2.2
1	В	225	ALA	2.2
1	В	124	TYR	2.2
1	А	573	ALA	2.2
1	В	215	LEU	2.2
1	В	560	GLU	2.2
1	В	577	ASN	2.2
1	В	212	VAL	2.2
1	В	620	LYS	2.2
1	В	103	GLY	2.2
1	В	36	LYS	2.1
1	A	230	ASN	2.1
1	В	34	GLY	2.1
1	В	59	ASP	2.1
1	В	178	ARG	2.1
1	В	210	ALA	2.1
1	В	164	ILE	2.1
1	В	74	GLU	2.0
1	В	553	VAL	2.0

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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 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	CL	А	701	1/1	0.95	0.12	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.

