



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:12 PM UTC

PDB ID : 8BZ4 / pdb_00008bz4
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 ⓘ 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

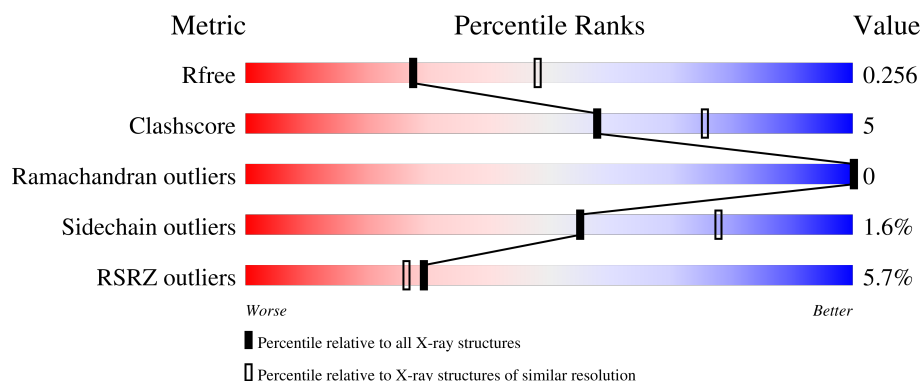
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (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 $\leq 5\%$. 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	624	89% 8% .
1	B	624	9% 77% 15% 8% .

2 Entry composition

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	A	606	Total	C	N	O	S	Se	0	1	0
			4915	3132	817	954	1	11			
1	B	577	Total	C	N	O	S	Se	16	0	0
			4691	2999	780	900	1	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A401AAP7
B	0	GLY	-	expression tag	UNP A0A401AAP7

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total	O	0	0
			206	206		
3	B	35	Total	O	0	0
			35	35		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.43Å 103.69Å 178.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 2.52 49.78 – 2.52	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.78-2.52) 100.0 (49.78-2.52)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.251 0.224 , 0.256	Depositor DCC
R_{free} test set	2573 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 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	A	0.20	0/5005	0.33	0/6741
1	B	0.19	0/4774	0.33	0/6423
All	All	0.19	0/9779	0.33	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

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	4915	0	4849	29	0
1	B	4691	0	4647	57	0
2	A	1	0	0	0	0
3	A	206	0	0	2	0
3	B	35	0	0	0	0
All	All	9848	0	9496	86	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 5.

All (86) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASP:CG	1:A:68:ARG:HH22	2.22	0.47
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:370:ASP:CG	1:A:484:ARG:HH22	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LYS:O	1:A:245:ILE:HG13	2.22	0.40
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

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	605/624 (97%)	585 (97%)	20 (3%)	0	100	100
1	B	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	Percentiles	
1	A	538/541 (99%)	535 (99%)	3 (1%)	78	90
1	B	513/541 (95%)	499 (97%)	14 (3%)	39	65
All	All	1051/1082 (97%)	1034 (98%)	17 (2%)	55	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ARG
1	A	536	LEU
1	A	621	ILE
1	B	27	THR
1	B	58	ASP
1	B	69	LEU
1	B	79	MSE
1	B	99	LYS
1	B	189	ASP
1	B	266	LEU
1	B	382	ARG
1	B	385	ARG
1	B	490	LYS
1	B	497	LEU
1	B	501	LYS
1	B	582	LEU
1	B	623	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	143	ASN
1	A	246	ASN
1	A	259	GLN
1	A	587	ASN
1	B	45	GLN
1	B	268	HIS
1	B	312	ASN
1	B	605	HIS

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 [i](#)

There are no oligosaccharides 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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	595/624 (95%)	-0.06	9 (1%) 72 69	24, 49, 85, 149	1 (0%)
1	B	566/624 (90%)	0.83	57 (10%) 12 10	50, 90, 150, 193	3 (0%)
All	All	1161/1248 (93%)	0.37	66 (5%) 29 26	24, 65, 139, 193	4 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	ILE	5.2
1	B	35	LEU	4.5
1	B	569	GLY	4.0
1	B	576	ILE	4.0
1	B	69	LEU	3.8
1	B	235	GLY	3.6
1	B	30	THR	3.5
1	B	574	ASP	3.4
1	B	91	SER	3.4
1	B	182	LEU	3.2
1	B	166	CYS	3.2
1	B	68	ARG	3.2
1	B	572	ASP	3.2
1	B	107	LEU	3.2
1	A	226	THR	3.1
1	B	225	ALA	3.1
1	A	572	ASP	3.1
1	B	28	TYR	3.1
1	A	573	ALA	3.1
1	B	25	VAL	3.0
1	B	23	VAL	2.9
1	B	595	LEU	2.9
1	B	108	TYR	2.8
1	B	621	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	2.8
1	B	540	THR	2.8
1	B	571	SER	2.7
1	B	34	GLY	2.7
1	A	227	GLY	2.7
1	B	81	VAL	2.7
1	A	569	GLY	2.6
1	B	575	PRO	2.6
1	B	565	LEU	2.6
1	B	176	TYR	2.6
1	B	56	PHE	2.6
1	B	195	LEU	2.6
1	B	593	VAL	2.6
1	B	46	THR	2.5
1	B	40	ALA	2.5
1	B	606	LEU	2.5
1	B	586	ALA	2.5
1	B	217	ASP	2.4
1	B	120	PHE	2.4
1	B	201	PHE	2.4
1	B	24	VAL	2.4
1	B	181	LEU	2.3
1	B	413	PRO	2.3
1	B	599	LYS	2.3
1	B	106	ILE	2.3
1	A	18	ASP	2.3
1	B	189	ASP	2.3
1	A	230	ASN	2.3
1	B	93	PRO	2.3
1	B	192	ALA	2.2
1	B	42	ILE	2.2
1	A	190	ASP	2.2
1	B	402	TYR	2.1
1	B	216	ALA	2.1
1	B	605	HIS	2.1
1	B	426	ILE	2.1
1	B	568	VAL	2.1
1	B	75	THR	2.0
1	B	476	THR	2.0
1	B	77	PRO	2.0
1	B	601	SER	2.0
1	B	579	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	CL	A	701	1/1	0.97	0.05	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.