



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2026 – 06:10 PM JST

PDB ID : 9VVT / pdb\_00009vvt  
Title : Crystal structure of the LysR-type transcriptional regulator CutR from mycobacterium sp. strain JC1  
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Deposited on : 2025-07-16  
Resolution : 2.50 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](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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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

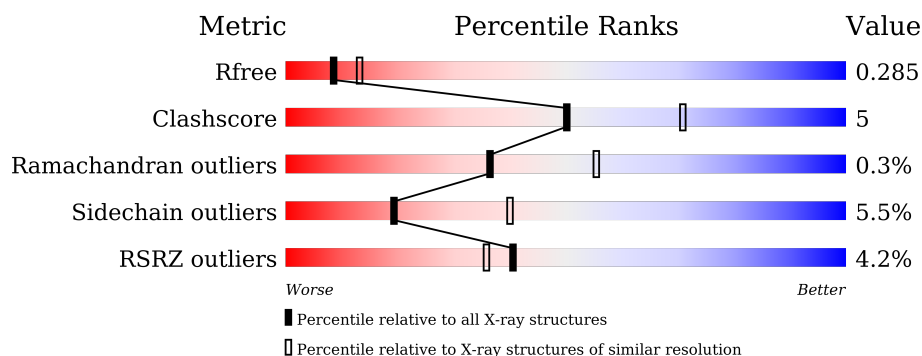
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	326	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	326	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4933 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 LysR family transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	Se	0	1	0
			2433	1529	454	442	2	6			
1	B	326	Total	C	N	O	S	Se	0	0	0
			2456	1542	460	446	2	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	HIS	-	expression tag	UNP D5G1X9
A	322	HIS	-	expression tag	UNP D5G1X9
A	323	HIS	-	expression tag	UNP D5G1X9
A	324	HIS	-	expression tag	UNP D5G1X9
A	325	HIS	-	expression tag	UNP D5G1X9
A	326	HIS	-	expression tag	UNP D5G1X9
B	321	HIS	-	expression tag	UNP D5G1X9
B	322	HIS	-	expression tag	UNP D5G1X9
B	323	HIS	-	expression tag	UNP D5G1X9
B	324	HIS	-	expression tag	UNP D5G1X9
B	325	HIS	-	expression tag	UNP D5G1X9
B	326	HIS	-	expression tag	UNP D5G1X9

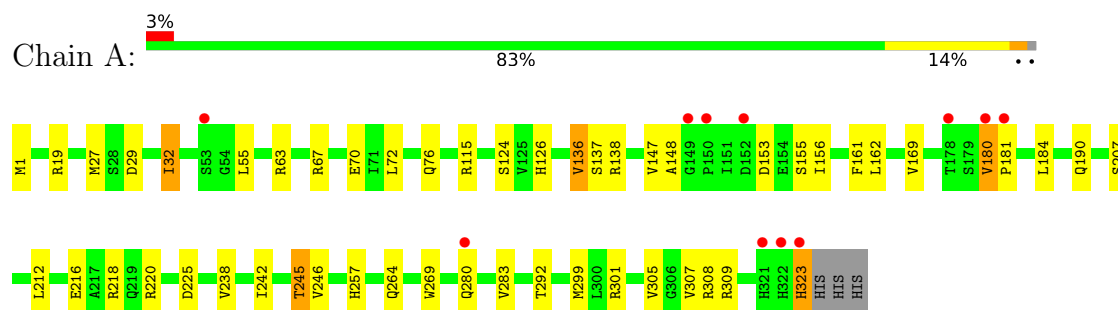
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	15	Total	O	0	0
			15	15		

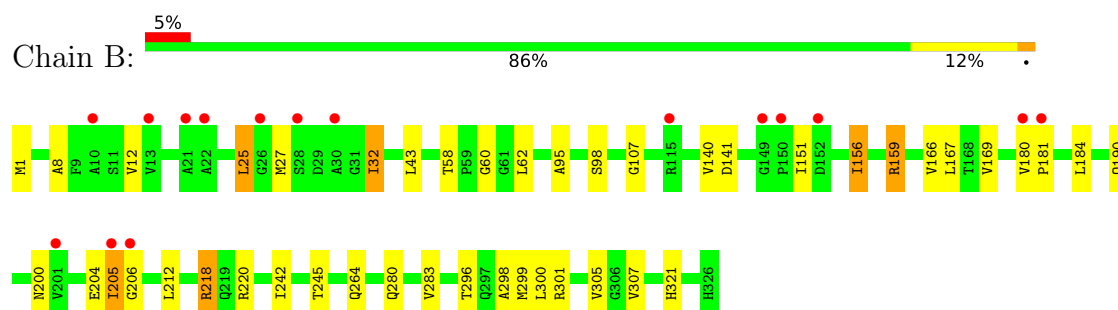
### 3 Residue-property plots [i](#)

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: LysR family transcriptional regulator



- Molecule 1: LysR family transcriptional regulator



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.50Å 92.08Å 126.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.26 – 2.50 40.26 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.26-2.50) 93.0 (40.26-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	49.08 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.212 , 0.268 0.237 , 0.285	Depositor DCC
$R_{free}$ test set	1252 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 26.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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	0.52	0/2476	0.84	1/3354 (0.0%)
1	B	0.52	0/2499	0.87	0/3385
All	All	0.52	0/4975	0.85	1/6739 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASP	N-CA-C	5.67	117.54	111.36

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2433	0	2508	27	0
1	B	2456	0	2516	28	0
2	A	29	0	0	1	0
2	B	15	0	0	0	0
All	All	4933	0	5024	52	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 (52) 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:205:ILE:HG12	1:B:205:ILE:O	1.66	0.95
1:A:136:VAL:HG23	1:A:156:ILE:HD11	1.67	0.76
1:A:245:THR:HA	1:A:299:MSE:HE1	1.66	0.76
1:B:27:MSE:HE3	1:B:32:ILE:HG12	1.72	0.70
1:B:280:GLN:HB2	1:B:283:VAL:HG23	1.75	0.68
1:A:307:VAL:HG12	1:A:308:ARG:HG3	1.76	0.68
1:A:245:THR:HG22	1:A:246:VAL:HG13	1.79	0.65
1:B:159:ARG:CG	1:B:159:ARG:HH21	2.10	0.64
1:A:180:VAL:HB	1:A:181:PRO:HD3	1.81	0.63
1:B:296:THR:HA	1:B:299:MSE:HE2	1.81	0.62
1:B:204:GLU:HG3	1:B:242:ILE:HD11	1.84	0.59
1:B:190:GLN:O	1:B:218:ARG:HG3	2.03	0.58
1:A:280:GLN:HB2	1:A:283:VAL:HG23	1.87	0.56
1:B:180:VAL:HB	1:B:181:PRO:CD	2.36	0.56
1:B:159:ARG:HH21	1:B:159:ARG:HG2	1.72	0.54
1:B:242:ILE:O	1:B:245:THR:HB	2.08	0.54
1:B:25:LEU:CD1	1:B:27:MSE:HE2	2.38	0.53
1:B:1:MSE:HE2	1:B:43:LEU:HD21	1.90	0.52
1:A:242:ILE:O	1:A:245:THR:HB	2.12	0.50
1:A:309:ARG:NH2	1:B:321:HIS:HA	2.27	0.49
1:B:159:ARG:CG	1:B:159:ARG:NH2	2.72	0.49
1:B:8:ALA:O	1:B:12:VAL:HG23	2.13	0.48
1:B:58:THR:HG22	1:B:60:GLY:H	1.78	0.48
1:A:124:SER:HB3	1:A:126:HIS:CE1	2.49	0.48
1:A:190:GLN:O	1:A:218:ARG:HD3	2.14	0.48
1:B:166:VAL:O	1:B:264:GLN:HA	2.14	0.48
1:A:257:HIS:CE1	1:A:264:GLN:OE1	2.67	0.48
1:A:72:LEU:O	1:A:76:GLN:HG2	2.14	0.48
1:B:25:LEU:HD13	1:B:27:MSE:HE2	1.96	0.47
1:A:216:GLU:HB3	1:B:307:VAL:HG21	1.96	0.47
1:A:162:LEU:HD22	1:A:269:TRP:CE3	2.49	0.47
1:B:141:ASP:HB3	1:B:283:VAL:CG2	2.45	0.47
1:B:184:LEU:HD21	1:B:212:LEU:HD22	1.97	0.46
1:A:301:ARG:NH2	2:A:402:HOH:O	2.47	0.46
1:B:95:ALA:HB2	1:B:140:VAL:HG11	1.97	0.46
1:B:298:ALA:HA	1:B:301:ARG:HD2	1.99	0.45
1:A:27:MSE:SE	1:A:32:ILE:HD12	2.67	0.45
1:A:67:ARG:NH2	1:A:70:GLU:OE1	2.50	0.45
1:A:323:HIS:ND1	1:A:323:HIS:C	2.74	0.45
1:A:115:ARG:H	1:A:115:ARG:HG2	1.67	0.44
1:A:245:THR:HA	1:A:299:MSE:CE	2.42	0.44
1:A:137:SER:O	1:A:138:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HB	1:A:181:PRO:CD	2.47	0.44
1:B:141:ASP:HB3	1:B:283:VAL:HG22	2.00	0.43
1:A:309:ARG:HH21	1:B:321:HIS:HA	1.82	0.43
1:B:151:ILE:HG21	1:B:156:ILE:HD11	2.00	0.42
1:A:19:ARG:NH1	1:A:29:ASP:OD2	2.53	0.42
1:A:153:ASP:OD2	1:A:155:SER:OG	2.38	0.42
1:B:107:GLY:HA3	1:B:298:ALA:O	2.21	0.40
1:A:161:PHE:CZ	1:A:269:TRP:HB3	2.57	0.40
1:A:184:LEU:HD21	1:A:212:LEU:HD22	2.02	0.40
1:B:167:LEU:HD23	1:B:264:GLN:HB2	2.04	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	322/326 (99%)	307 (95%)	14 (4%)	1 (0%)	36	55
1	B	324/326 (99%)	309 (95%)	14 (4%)	1 (0%)	36	55
All	All	646/652 (99%)	616 (95%)	28 (4%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	B	206	GLY

### 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	255/251 (102%)	239 (94%)	16 (6%)	16	34
1	B	257/251 (102%)	244 (95%)	13 (5%)	21	43
All	All	512/502 (102%)	483 (94%)	29 (6%)	19	39

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	32	ILE
1	A	55	LEU
1	A	63	ARG
1	A	136	VAL
1	A	147	VAL
1	A	169	VAL
1	A	180	VAL
1	A	207	SER
1	A	220[A]	ARG
1	A	220[B]	ARG
1	A	238	VAL
1	A	245	THR
1	A	292	THR
1	A	305	VAL
1	A	323	HIS
1	B	25	LEU
1	B	32	ILE
1	B	62	LEU
1	B	98	SER
1	B	156	ILE
1	B	159	ARG
1	B	169	VAL
1	B	200	ASN
1	B	205	ILE
1	B	218	ARG
1	B	220	ARG
1	B	300	LEU
1	B	305	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	126	HIS
1	A	233	GLN
1	A	257	HIS
1	B	233	GLN
1	B	326	HIS

### 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](#)

There are no ligands in this entry.

## 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<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	317/326 (97%)	0.34	11 (3%) 47 42	19, 36, 43, 47	1 (0%)
1	B	320/326 (98%)	0.49	16 (5%) 34 30	25, 37, 56, 62	0
All	All	637/652 (97%)	0.41	27 (4%) 40 36	19, 37, 50, 62	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	ASP	3.5
1	A	181	PRO	3.5
1	A	178	THR	3.3
1	B	30	ALA	3.3
1	A	180	VAL	3.2
1	B	150	PRO	3.2
1	B	205	ILE	3.1
1	B	180	VAL	2.9
1	A	323	HIS	2.9
1	A	152	ASP	2.8
1	A	150	PRO	2.6
1	A	53	SER	2.6
1	A	149	GLY	2.6
1	B	201	VAL	2.5
1	B	181	PRO	2.5
1	B	22	ALA	2.4
1	B	13	VAL	2.4
1	B	28	SER	2.3
1	B	21	ALA	2.3
1	A	321	HIS	2.2
1	B	26	GLY	2.2
1	B	206	GLY	2.2
1	B	149	GLY	2.2
1	A	280	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	2.0
1	B	115	ARG	2.0
1	A	322	HIS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.