



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2026 – 08:11 AM EDT

PDB ID : 12AJ / pdb\_000012aj  
Title : Citrobacter rodentium contact dependent growth inhibition (CDI) toxin (CdiA-CT) in complex with E. coli GyrB  
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Deposited on : 2026-03-23  
Resolution : 2.00 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)

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<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	:	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

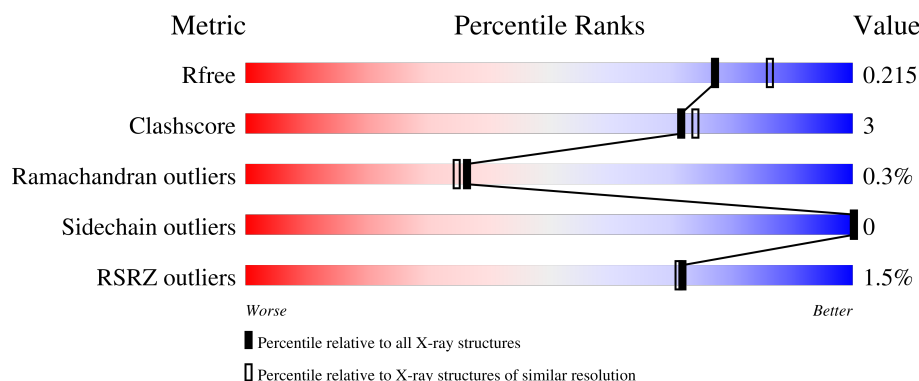
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	B	230	 79% 8% 13%
2	A	164	 2% 82% 14%

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
3	GOL	B	305	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2760 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 DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	200	Total	C	N	O	S	0	5	0
			1562	984	277	295	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP A0A7D7JXT0
B	1	ALA	-	expression tag	UNP A0A7D7JXT0
B	222	LEU	-	expression tag	UNP A0A7D7JXT0
B	223	GLU	-	expression tag	UNP A0A7D7JXT0
B	224	HIS	-	expression tag	UNP A0A7D7JXT0
B	225	HIS	-	expression tag	UNP A0A7D7JXT0
B	226	HIS	-	expression tag	UNP A0A7D7JXT0
B	227	HIS	-	expression tag	UNP A0A7D7JXT0
B	228	HIS	-	expression tag	UNP A0A7D7JXT0
B	229	HIS	-	expression tag	UNP A0A7D7JXT0

- Molecule 2 is a protein called Contact-dependent inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	141	Total	C	N	O	S	0	0	0
			1025	643	172	204	6			

There are 22 discrepancies between the modelled and reference sequences:

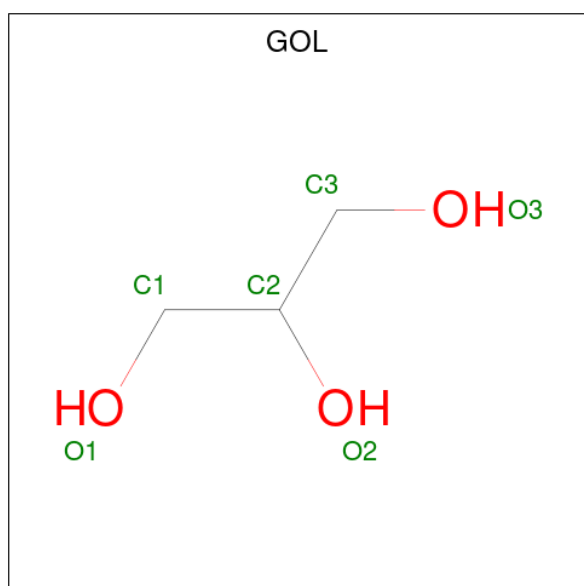
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	initiating methionine	UNP A0A482PFX0
A	139	HIS	-	expression tag	UNP A0A482PFX0
A	140	HIS	-	expression tag	UNP A0A482PFX0
A	141	HIS	-	expression tag	UNP A0A482PFX0
A	142	HIS	-	expression tag	UNP A0A482PFX0
A	143	HIS	-	expression tag	UNP A0A482PFX0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	144	HIS	-	expression tag	UNP A0A482PFX0
A	145	SER	-	expression tag	UNP A0A482PFX0
A	146	SER	-	expression tag	UNP A0A482PFX0
A	147	GLY	-	expression tag	UNP A0A482PFX0
A	148	VAL	-	expression tag	UNP A0A482PFX0
A	149	ASP	-	expression tag	UNP A0A482PFX0
A	150	LEU	-	expression tag	UNP A0A482PFX0
A	151	GLY	-	expression tag	UNP A0A482PFX0
A	152	THR	-	expression tag	UNP A0A482PFX0
A	153	GLU	-	expression tag	UNP A0A482PFX0
A	154	ASN	-	expression tag	UNP A0A482PFX0
A	155	LEU	-	expression tag	UNP A0A482PFX0
A	156	TYR	-	expression tag	UNP A0A482PFX0
A	157	PHE	-	expression tag	UNP A0A482PFX0
A	158	GLN	-	expression tag	UNP A0A482PFX0
A	183	ALA	CYS	engineered mutation	UNP A0A482PFX0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

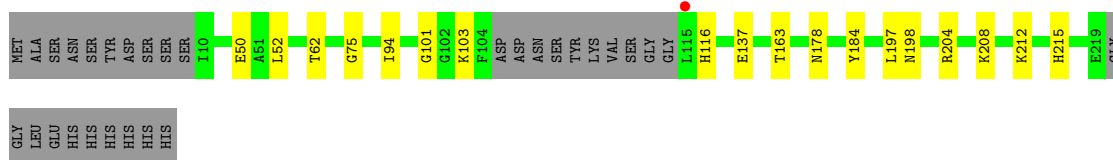
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	98	Total	O	0	0
			98	98		
4	A	33	Total	O	0	0
			33	33		

### 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.

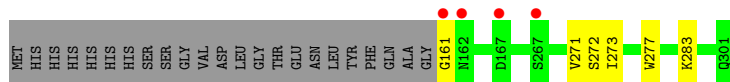
- Molecule 1: DNA gyrase subunit B

Chain B: 



- Molecule 2: Contact-dependent inhibitor A

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.45Å 64.95Å 70.15Å 90.00° 101.69° 90.00°	Depositor
Resolution (Å)	35.69 – 2.00 35.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (35.69-2.00) 98.3 (35.69-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.175 , 0.215 0.175 , 0.215	Depositor DCC
$R_{free}$ test set	2147 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	B	0.24	0/1610	0.40	0/2179
2	A	0.18	0/1051	0.38	0/1431
All	All	0.22	0/2661	0.39	0/3610

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	B	1562	0	1527	15	0
2	A	1025	0	908	4	0
3	A	6	0	8	0	0
3	B	36	0	48	5	0
4	A	33	0	0	0	0
4	B	98	0	0	0	0
All	All	2760	0	2491	17	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 3.

All (17) 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:163:THR:CG2	3:B:305:GOL:H32	2.28	0.64
1:B:163:THR:HG22	3:B:305:GOL:H32	1.80	0.62
1:B:184:TYR:CE1	1:B:212:LYS:HD3	2.39	0.57
2:A:271:VAL:HG13	2:A:273:ILE:HD11	1.85	0.57
1:B:50:GLU:HG2	1:B:75:GLY:HA3	1.87	0.56
2:A:272:SER:HB2	2:A:283:LYS:NZ	2.25	0.51
1:B:103:LYS:HD3	2:A:161:GLY:HA3	1.94	0.49
1:B:103:LYS:HD2	2:A:277:TRP:CD1	2.49	0.48
1:B:197:LEU:O	3:B:304:GOL:H12	2.12	0.48
1:B:204:ARG:NH2	1:B:215:HIS:CE1	2.82	0.48
1:B:137:GLU:N	3:B:305:GOL:H31	2.29	0.48
1:B:52:LEU:HG	1:B:198:ASN:HD21	1.79	0.47
1:B:62:THR:HG21	1:B:208:LYS:HE2	2.00	0.44
1:B:184:TYR:CZ	1:B:212:LYS:HD3	2.55	0.42
1:B:137:GLU:H	3:B:305:GOL:H31	1.84	0.41
1:B:94:ILE:HD13	1:B:116:HIS:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	B	202/230 (88%)	199 (98%)	2 (1%)	1 (0%)	24	21
2	A	139/164 (85%)	136 (98%)	3 (2%)	0	100	100
All	All	341/394 (86%)	335 (98%)	5 (2%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	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	B	167/193 (86%)	167 (100%)	0	100	100
2	A	99/133 (74%)	99 (100%)	0	100	100
All	All	266/326 (82%)	266 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	GLN
1	B	198	ASN
1	B	217	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](#)

7 ligands are 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
3	GOL	B	303	-	5,5,5	0.33	0	5,5,5	0.24	0
3	GOL	B	301	-	5,5,5	0.35	0	5,5,5	0.42	0
3	GOL	B	300	-	5,5,5	0.35	0	5,5,5	0.48	0
3	GOL	B	304	-	5,5,5	0.38	0	5,5,5	0.60	0
3	GOL	A	401	-	5,5,5	0.33	0	5,5,5	0.43	0
3	GOL	B	305	-	5,5,5	0.34	0	5,5,5	0.47	0
3	GOL	B	302	-	5,5,5	0.30	0	5,5,5	0.38	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
3	GOL	B	303	-	-	2/4/4/4	-
3	GOL	B	301	-	-	0/4/4/4	-
3	GOL	B	300	-	-	0/4/4/4	-
3	GOL	B	304	-	-	0/4/4/4	-
3	GOL	A	401	-	-	2/4/4/4	-
3	GOL	B	305	-	-	1/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	C1-C2-C3-O3
3	B	303	GOL	C1-C2-C3-O3
3	B	303	GOL	O2-C2-C3-O3
3	A	401	GOL	O2-C2-C3-O3
3	B	305	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	304	GOL	1	0
3	B	305	GOL	4	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	B	200/230 (86%)	-0.18	1 (0%) 87 87	11, 30, 52, 73	5 (2%)
2	A	141/164 (85%)	0.18	4 (2%) 55 54	23, 41, 60, 81	0
All	All	341/394 (86%)	-0.03	5 (1%) 72 71	11, 34, 60, 81	5 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	267	SER	2.4
1	B	115	LEU	2.3
2	A	167	ASP	2.3
2	A	161	GLY	2.3
2	A	162	ASN	2.2

### 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	305	6/6	0.54	0.18	37,42,44,53	6
3	GOL	A	401	6/6	0.74	0.15	51,59,62,64	0
3	GOL	B	302	6/6	0.75	0.17	45,47,49,52	6
3	GOL	B	303	6/6	0.75	0.13	51,56,61,69	0
3	GOL	B	300	6/6	0.80	0.15	43,52,58,63	6
3	GOL	B	304	6/6	0.81	0.18	36,42,44,59	6
3	GOL	B	301	6/6	0.84	0.11	41,46,48,50	6

## 6.5 Other polymers [i](#)

There are no such residues in this entry.