



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2025 – 04:07 PM EDT

PDB ID : 9MTV / pdb\_00009mtv  
Title : Crystal structure of an apo-ADC-1 triple mutant  
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Deposited on : 2025-01-12  
Resolution : 1.80 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

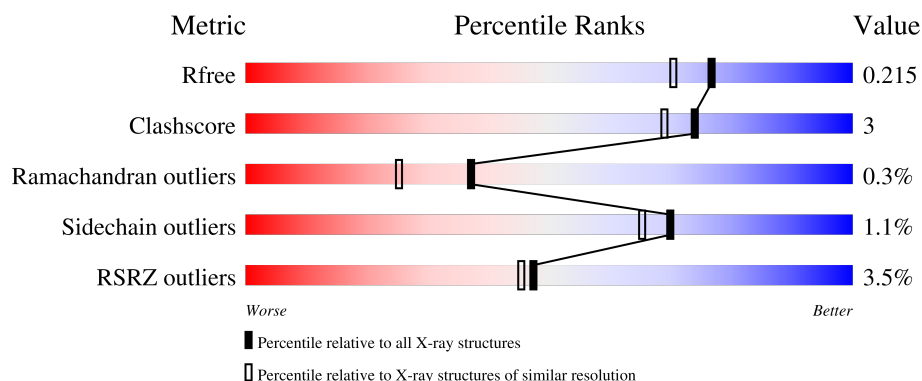
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	360	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	360	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6016 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.

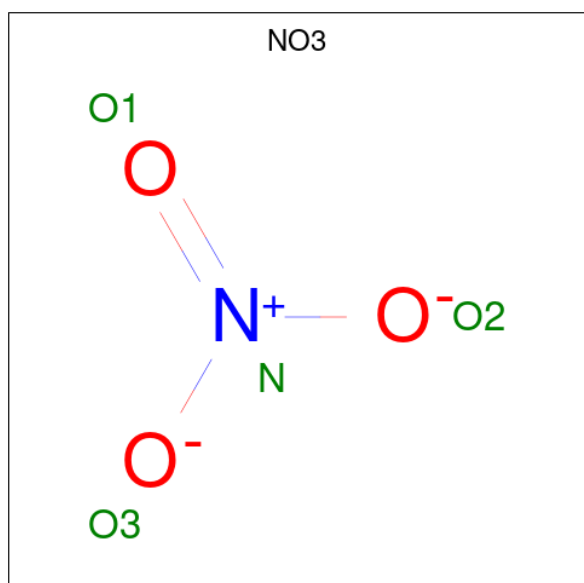
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	5	0
			2886	1853	482	541	10			
1	B	353	Total	C	N	O	S	0	1	0
			2812	1806	467	530	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	PHE	VAL	engineered mutation	UNP Q9L4R5
A	317	THR	SER	engineered mutation	UNP Q9L4R5
A	321	SER	PHE	engineered mutation	UNP Q9L4R5
B	294	PHE	VAL	engineered mutation	UNP Q9L4R5
B	317	THR	SER	engineered mutation	UNP Q9L4R5
B	321	SER	PHE	engineered mutation	UNP Q9L4R5

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

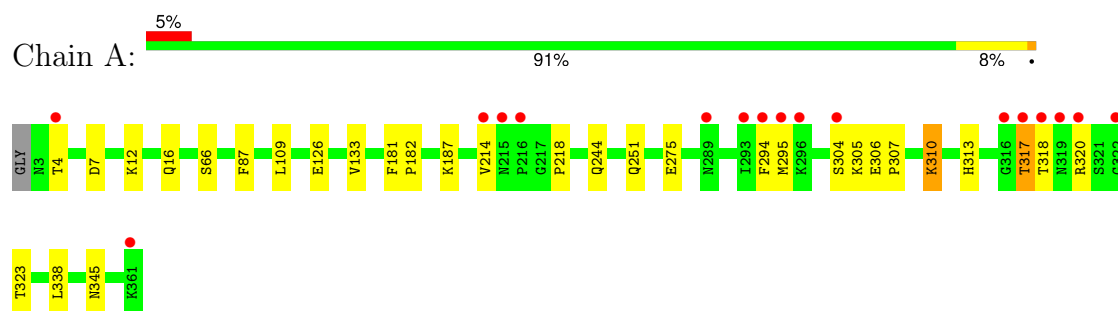
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	1
			182	182		
4	B	124	Total	O	0	0
			124	124		

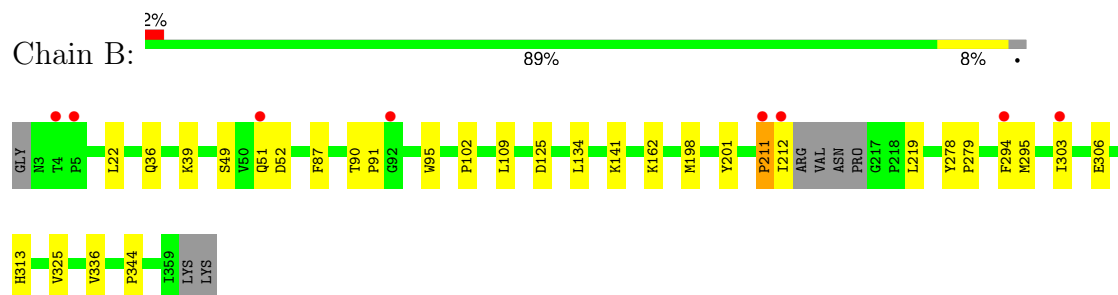
### 3 Residue-property plots

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: Beta-lactamase



#### • Molecule 1: Beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.09Å 182.21Å 50.77Å 90.00° 99.41° 90.00°	Depositor
Resolution (Å)	38.64 – 1.80 38.64 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.64-1.80) 98.9 (38.64-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.187 , 0.215 0.187 , 0.215	Depositor DCC
$R_{free}$ test set	3444 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NO3, EDO

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	0.41	0/2968	0.55	0/4019
1	B	0.39	0/2880	0.55	2/3901 (0.1%)
All	All	0.40	0/5848	0.55	2/7920 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	211	PRO	CB-CA-C	-5.02	99.44	112.00

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	2886	0	2914	17	0
1	B	2812	0	2821	17	0
2	B	4	0	0	0	0
3	B	8	0	12	1	0
4	A	182	0	0	0	0
4	B	124	0	0	1	0
All	All	6016	0	5747	34	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 (34) 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:344:PRO:HD3	3:B:402:EDO:H11	1.68	0.75
1:A:317:THR:HG22	1:A:345:ASN:HD21	1.53	0.71
1:A:317:THR:OG1	1:A:318:THR:N	2.30	0.65
1:B:36:GLN:O	1:B:39:LYS:HE2	1.98	0.64
1:B:294:PHE:HD2	1:B:295:MET:HG2	1.67	0.59
1:A:306[A]:GLU:HG2	1:A:307:PRO:HD2	1.85	0.57
1:A:214:VAL:HG12	1:A:320:ARG:HH22	1.68	0.57
1:A:126:GLU:N	1:A:126:GLU:OE2	2.36	0.56
1:B:198:MET:CE	1:B:212:ILE:HD13	2.37	0.55
1:A:133:VAL:HG21	1:A:218:PRO:HB2	1.90	0.53
1:B:201:TYR:CD1	1:B:212:ILE:HD11	2.46	0.51
1:B:303:ILE:HG12	4:B:514:HOH:O	2.11	0.50
1:A:87:PHE:HB3	1:A:109:LEU:HB2	1.94	0.49
1:B:198:MET:HE2	1:B:212:ILE:HD13	1.93	0.49
1:A:323:THR:HG23	1:A:338:LEU:HD23	1.94	0.49
1:A:126:GLU:H	1:A:126:GLU:CD	2.16	0.49
1:B:49:SER:OG	1:B:51:GLN:HG2	2.13	0.48
1:A:4:THR:N	1:A:7:ASP:OD2	2.42	0.47
1:B:278:TYR:CD1	1:B:279:PRO:HA	2.50	0.46
1:B:162:LYS:HD2	1:B:219:LEU:HD21	1.96	0.46
1:B:39:LYS:HB2	1:B:39:LYS:HE3	1.63	0.45
1:B:325:VAL:HG12	1:B:336:VAL:HG22	1.98	0.45
1:B:87:PHE:HB3	1:B:109:LEU:HB2	1.99	0.44
1:B:102:PRO:HG2	1:B:141:LYS:HD2	1.99	0.44
1:A:275:GLU:OE2	1:A:310:LYS:HG2	2.17	0.43
1:A:12:LYS:HG2	1:A:16:GLN:NE2	2.33	0.42
1:B:95:TRP:CZ2	1:B:134:LEU:HD13	2.55	0.41
1:A:304:SER:OG	1:A:305:LYS:N	2.51	0.41
1:A:294:PHE:CD2	1:A:295:MET:HG2	2.56	0.41
1:B:90:THR:HB	1:B:91:PRO:HD2	2.03	0.41
1:A:244:GLN:HA	1:A:251[A]:GLN:CD	2.41	0.41
1:A:187:LYS:HA	1:A:187:LYS:HD3	1.87	0.41
1:A:181:PHE:HB2	1:A:182:PRO:HD3	2.02	0.41
1:B:294:PHE:CD2	1:B:295:MET:HG2	2.52	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	A	362/360 (101%)	353 (98%)	8 (2%)	1 (0%)	37	25
1	B	350/360 (97%)	339 (97%)	10 (3%)	1 (0%)	37	25
All	All	712/720 (99%)	692 (97%)	18 (2%)	2 (0%)	37	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	THR
1	B	211	PRO

### 5.3.2 Protein sidechains

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	320/315 (102%)	317 (99%)	3 (1%)	75	72
1	B	310/315 (98%)	306 (99%)	4 (1%)	65	59
All	All	630/630 (100%)	623 (99%)	7 (1%)	70	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	310	LYS
1	A	313	HIS
1	B	22	LEU

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Mol	Chain	Res	Type
1	B	125	ASP
1	B	306	GLU
1	B	313	HIS

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	8	GLN
1	A	16	GLN
1	A	283	GLN
1	A	292	GLN
1	A	345	ASN
1	B	174	GLN

### 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](#)

3 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	EDO	B	403	-	3,3,3	0.31	0	2,2,2	0.26	0
3	EDO	B	402	-	3,3,3	0.27	0	2,2,2	0.33	0
2	NO3	B	401	-	1,3,3	0.09	0	0,3,3	-	-

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	EDO	B	403	-	-	0/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	EDO	1	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

### 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	359/360 (99%)	0.00	17 (4%) 37 34	13, 26, 59, 90	5 (1%)
1	B	353/360 (98%)	0.04	8 (2%) 61 59	16, 31, 57, 77	1 (0%)
All	All	712/720 (98%)	0.02	25 (3%) 47 45	13, 28, 57, 90	6 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	ILE	5.9
1	A	317	THR	5.2
1	A	294	PHE	4.8
1	A	318	THR	4.7
1	A	295	MET	3.4
1	A	319	ASN	3.3
1	B	211	PRO	3.3
1	A	322	GLY	3.2
1	A	214	VAL	2.9
1	B	5	PRO	2.7
1	A	316	GLY	2.7
1	A	215	ASN	2.6
1	A	289	ASN	2.4
1	B	4	THR	2.4
1	A	320	ARG	2.3
1	B	294	PHE	2.3
1	A	304	SER	2.3
1	A	293	ILE	2.3
1	A	216	PRO	2.2
1	A	4	THR	2.2
1	A	296	LYS	2.2
1	B	92	GLY	2.1
1	B	51	GLN	2.1
1	A	361	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	303	ILE	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 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<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
3	EDO	B	402	4/4	0.84	0.15	38,39,40,42	0
3	EDO	B	403	4/4	0.88	0.13	30,30,35,36	0
2	NO3	B	401	4/4	0.94	0.12	34,39,39,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.