



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2025 – 12:39 PM EDT

PDB ID : 9EA5 / pdb_00009ea5
Title : Structure of Citrobacter BubCD D104A mutant
Authors : Ye, Q.; Corbett, K.D.
Deposited on : 2024-11-10
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

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 Phenix2.0rc1
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) : 2.45.1

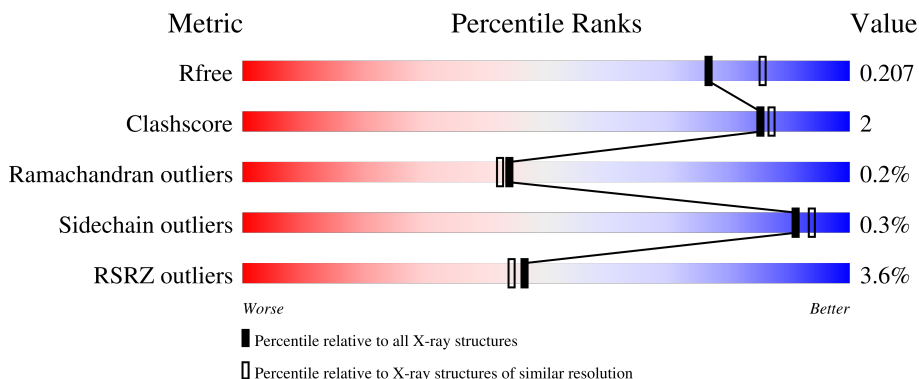
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

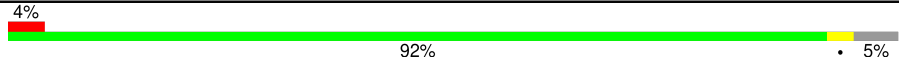
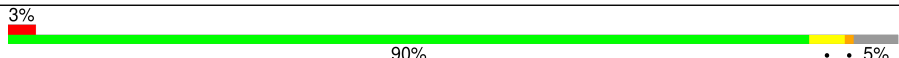
The reported resolution of this entry is 2.00 Å.

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 ≥ 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	458	 4% 92% 5%
1	B	458	 3% 90% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14201 atoms, of which 6752 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.

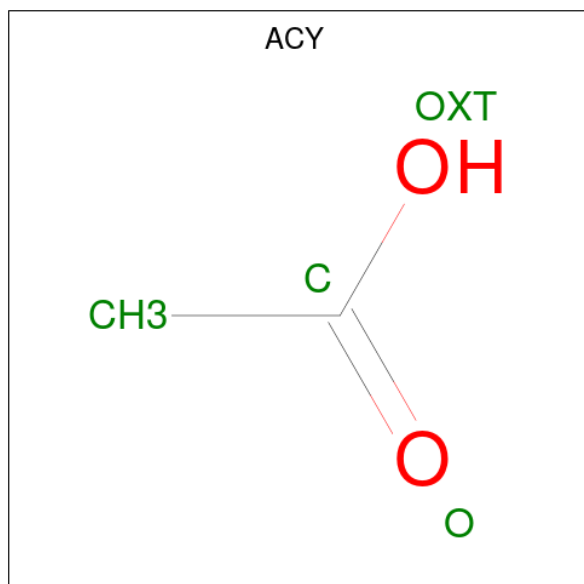
- Molecule 1 is a protein called Citrobacter BubCD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6767	2141	3378	583	648	17			
1	B	434	Total	C	H	N	O	S	0	0	0
			6738	2132	3365	580	644	17			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0

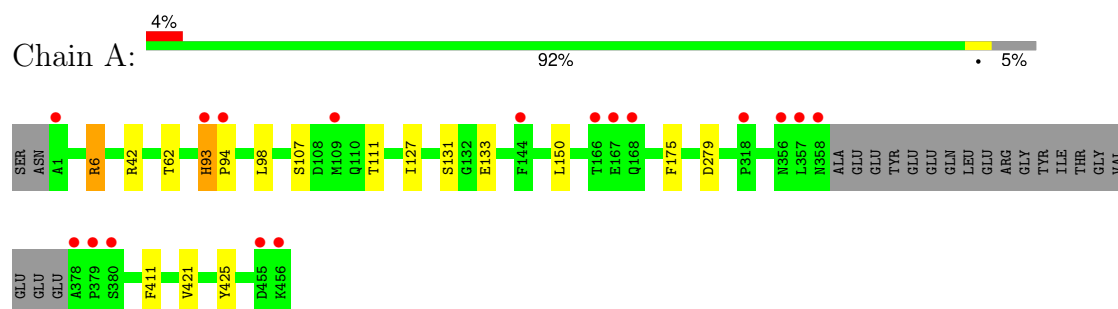
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	354	Total O 354 354	0	0
4	B	319	Total O 319 319	0	0

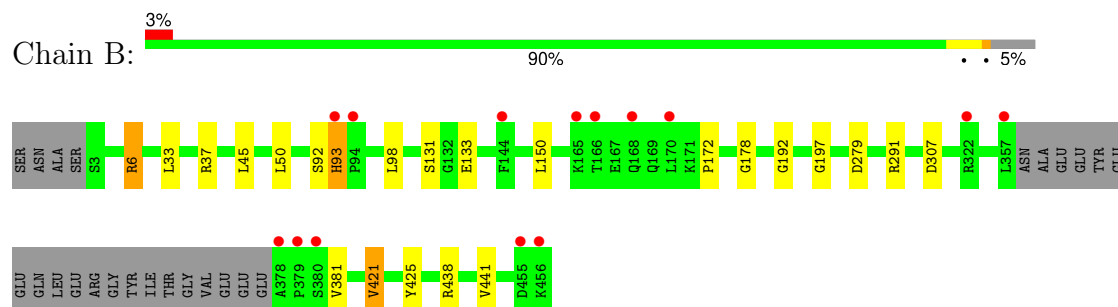
3 Residue-property plots [i](#)

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: Citrobacter BubCD



• Molecule 1: Citrobacter BubCD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.87Å 73.06Å 98.40Å 90.00° 108.72° 90.00°	Depositor
Resolution (Å)	39.29 – 2.00 39.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.29-2.00) 98.7 (39.29-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.172 , 0.207 0.172 , 0.207	Depositor DCC
R_{free} test set	2805 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14201	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8982e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/3450	0.33	0/4669
1	B	0.12	0/3434	0.31	0/4647
All	All	0.12	0/6884	0.32	0/9316

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	ARG	Sidechain
1	B	6	ARG	Sidechain

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	3389	3378	3380	15	0
1	B	3373	3365	3365	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	3	3	0	0
3	B	8	6	6	1	0
4	A	354	0	0	1	1
4	B	319	0	0	0	2
All	All	7449	6752	6754	28	3

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 2.

All (28) 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:A:131:SER:OG	1:A:133:GLU:OE1	2.02	0.76
1:B:131:SER:OG	1:B:133:GLU:OE1	2.11	0.61
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.71	0.56
1:B:98:LEU:C	1:B:98:LEU:HD12	2.34	0.53
1:A:93:HIS:HB3	1:A:94:PRO:HD3	1.91	0.53
1:A:421:VAL:HG12	1:A:421:VAL:O	2.09	0.53
1:A:6:ARG:HD3	1:A:150:LEU:HD23	1.89	0.53
1:A:93:HIS:O	1:A:94:PRO:C	2.51	0.52
1:A:98:LEU:C	1:A:98:LEU:HD12	2.35	0.52
1:A:62:THR:HG23	4:A:732:HOH:O	2.10	0.51
1:A:411:PHE:CZ	1:B:421:VAL:HG21	2.46	0.49
1:B:438:ARG:O	1:B:441:VAL:HG22	2.14	0.48
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.80	0.47
1:B:291:ARG:NH1	1:B:307:ASP:OD1	2.42	0.47
1:A:6:ARG:NE	1:A:279:ASP:OD1	2.49	0.46
1:B:6:ARG:HD3	1:B:150:LEU:HD23	1.98	0.45
1:B:33:LEU:HD13	1:B:50:LEU:HD13	1.99	0.44
1:A:93:HIS:HA	1:A:127:ILE:HG23	1.99	0.44
1:B:192:GLY:O	1:B:197:GLY:HA3	2.18	0.43
1:B:37:ARG:HG2	1:B:45:LEU:HD23	2.00	0.43
1:A:421:VAL:CG1	1:B:425:TYR:CE2	3.02	0.43
1:A:175:PHE:CD1	1:B:381:VAL:HG11	2.55	0.42
1:B:172:PRO:HB3	1:B:178:GLY:HA3	2.01	0.42
1:B:133:GLU:O	3:B:603:ACY:H3	2.20	0.42
1:B:92:SER:O	1:B:93:HIS:C	2.63	0.41
1:A:107:SER:O	1:A:111:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:NE	1:B:279:ASP:OD1	2.53	0.41
1:A:425:TYR:CE2	1:B:421:VAL:HG12	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:825:HOH:O	4:B:979:HOH:O[1_455]	2.14	0.06
4:B:827:HOH:O	4:B:952:HOH:O[1_655]	2.18	0.02
4:A:901:HOH:O	4:A:908:HOH:O[2_645]	2.19	0.01

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	433/458 (94%)	418 (96%)	14 (3%)	1 (0%)	44	42
1	B	430/458 (94%)	418 (97%)	11 (3%)	1 (0%)	44	42
All	All	863/916 (94%)	836 (97%)	25 (3%)	2 (0%)	44	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	B	93	HIS

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	366/387 (95%)	365 (100%)	1 (0%)	91	94
1	B	365/387 (94%)	364 (100%)	1 (0%)	91	94
All	All	731/774 (94%)	729 (100%)	2 (0%)	91	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	B	421	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	B	117	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	ACY	A	602	-	3,3,3	1.24	0	3,3,3	1.10	0
3	ACY	B	602	-	3,3,3	1.28	0	3,3,3	1.10	0
3	ACY	B	603	-	3,3,3	1.24	0	3,3,3	1.15	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	ACY	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, 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	437/458 (95%)	-0.24	17 (3%) 44 42	18, 29, 67, 135	0
1	B	434/458 (94%)	-0.16	14 (3%) 50 48	19, 32, 69, 114	0
All	All	871/916 (95%)	-0.20	31 (3%) 46 44	18, 31, 69, 135	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	ALA	4.5
1	A	358	ASN	4.2
1	B	380	SER	4.0
1	B	379	PRO	3.7
1	B	168	GLN	3.4
1	A	380	SER	3.4
1	A	318	PRO	3.0
1	B	170	LEU	2.9
1	B	456	LYS	2.8
1	A	93	HIS	2.8
1	B	93	HIS	2.8
1	B	94	PRO	2.7
1	A	167	GLU	2.7
1	B	166	THR	2.6
1	A	166	THR	2.5
1	B	357	LEU	2.5
1	A	168	GLN	2.5
1	A	356	ASN	2.4
1	A	357	LEU	2.4
1	A	144	PHE	2.3
1	A	109	MET	2.3
1	B	165	LYS	2.3
1	A	378	ALA	2.2
1	B	322	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	144	PHE	2.2
1	A	1	ALA	2.2
1	A	455	ASP	2.1
1	A	379	PRO	2.1
1	A	456	LYS	2.1
1	A	94	PRO	2.0
1	B	455	ASP	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(\AA^2)	Q<0.9
3	ACY	B	603	4/4	0.77	0.18	38,43,45,45	0
3	ACY	A	602	4/4	0.89	0.12	27,30,32,33	0
3	ACY	B	602	4/4	0.92	0.16	34,35,41,41	0
2	NA	B	601	1/1	0.93	0.05	32,32,32,32	0
2	NA	A	601	1/1	0.98	0.03	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.