



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7BK7  
Title : PfCopC mutant - D83N  
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Deposited on : 2021-01-15  
Resolution : 2.30 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.22  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.22

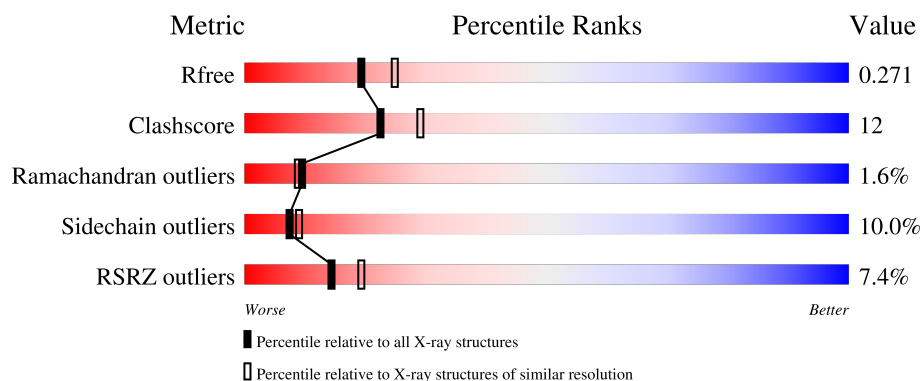
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	AAA	97	<div> <div>4%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	BBB	97	<div> <div>10%</div> <div>75%</div> <div>18%</div> <div>5%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 1574 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 Putative copper resistance protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	AAA	95	Total	C	N	O	0	7	0
			741	467	125	149			
1	BBB	95	Total	C	N	O	0	5	0
			741	469	127	145			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	83	ASN	ASP	engineered mutation	UNP C3JYL7
BBB	83	ASN	ASP	engineered mutation	UNP C3JYL7

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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

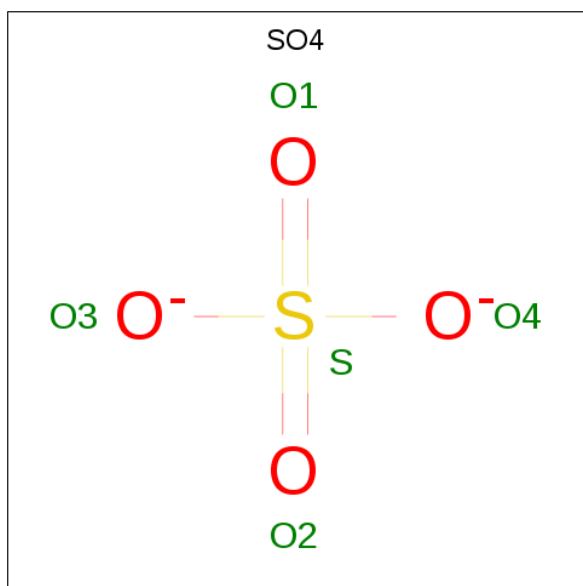
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Cu	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total	Cl	0	0
			2	2		
4	BBB	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	51	Total 52	O 52	0	1
6	BBB	23	Total 23	O 23	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.

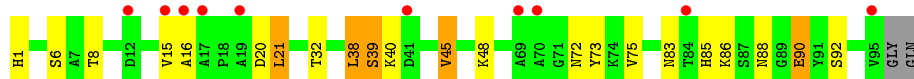
- Molecule 1: Putative copper resistance protein

Chain AAA:  4% 70% 26% ..



- Molecule 1: Putative copper resistance protein

Chain BBB:  10% 75% 18% 5% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.30 Å 80.30 Å 89.89 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.27 – 2.30 35.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.27-2.30) 99.9 (35.24-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.208 , 0.268 0.211 , 0.271	Depositor DCC
$R_{free}$ test set	647 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: ACT, SO4, CU, 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	AAA	0.71	0/756	0.87	0/1034
1	BBB	0.69	0/755	0.85	0/1028
All	All	0.70	0/1511	0.86	0/2062

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	AAA	741	0	740	24	0
1	BBB	741	0	754	12	0
2	AAA	4	0	3	1	0
2	BBB	4	0	3	0	0
3	AAA	1	0	0	0	0
4	AAA	2	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	5	0	0	0	0
6	AAA	52	0	0	3	0
6	BBB	23	0	0	0	0
All	All	1574	0	1500	35	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 12.

All (35) 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:BBB:38[B]:LEU:HB3	1:BBB:45:VAL:HG23	1.49	0.91
1:BBB:38[B]:LEU:CB	1:BBB:45:VAL:HG23	2.14	0.76
1:BBB:38[B]:LEU:HB3	1:BBB:45:VAL:CG2	2.20	0.71
1:AAA:22:ARG:HD3	2:AAA:201:ACT:H1	1.82	0.61
1:AAA:7[A]:ALA:O	1:AAA:8[A]:THR:HG22	2.02	0.59
1:AAA:70:ALA:HA	1:AAA:95:VAL:HB	1.85	0.58
1:AAA:9:PRO:HD2	1:AAA:21:LEU:HD22	1.87	0.57
1:BBB:15:VAL:CG1	1:BBB:16:ALA:N	2.69	0.55
1:AAA:8[A]:THR:O	1:AAA:8[A]:THR:HG23	2.09	0.53
1:BBB:1:HIS:NE2	1:BBB:85:HIS:CG	2.77	0.52
1:AAA:18[A]:PRO:O	1:AAA:19[A]:ALA:HB3	2.09	0.52
1:AAA:7[A]:ALA:O	1:AAA:8[A]:THR:HB	2.11	0.50
1:AAA:8[A]:THR:CG2	1:AAA:22:ARG:HB2	2.42	0.50
1:AAA:8[A]:THR:HA	1:AAA:9:PRO:C	2.32	0.49
1:AAA:84:THR:HG22	6:AAA:313:HOH:O	2.12	0.49
1:AAA:7[A]:ALA:O	1:AAA:8[A]:THR:CB	2.61	0.48
1:AAA:50:LEU:CD2	1:AAA:62:VAL:HG22	2.44	0.47
1:AAA:8[A]:THR:CA	1:AAA:9:PRO:C	2.83	0.47
1:BBB:38[B]:LEU:O	1:BBB:39[B]:SER:CB	2.63	0.46
1:AAA:7[A]:ALA:O	1:AAA:8[A]:THR:CG2	2.63	0.46
1:AAA:54:ASP:OD2	6:AAA:301:HOH:O	2.21	0.45
1:BBB:15:VAL:HG12	1:BBB:16:ALA:N	2.33	0.44
1:AAA:56:ASP:OD1	1:AAA:57:LYS:N	2.51	0.44
1:AAA:72:ASN:OD1	1:AAA:94:LYS:HG3	2.18	0.44
1:AAA:77:TRP:CD1	1:AAA:89[B]:GLY:O	2.72	0.43
1:BBB:20:ASP:C	1:BBB:21[A]:LEU:HD23	2.39	0.43
1:AAA:35:LYS:HA	1:BBB:32:THR:O	2.18	0.43
1:BBB:75:VAL:O	1:BBB:90:GLU:HA	2.18	0.43
1:AAA:83:ASN:O	1:AAA:84:THR:OG1	2.31	0.42
1:AAA:7[B]:ALA:O	1:AAA:10:ALA:HA	2.20	0.42
1:BBB:40:LYS:HB2	1:BBB:73:TYR:CE2	2.56	0.41
1:AAA:15:VAL:HG22	1:AAA:16:ALA:N	2.35	0.41
1:BBB:38[B]:LEU:HD13	1:BBB:38[B]:LEU:HA	1.76	0.41
1:AAA:18[A]:PRO:O	1:AAA:19[A]:ALA:CB	2.68	0.41
1:AAA:18[A]:PRO:HD2	6:AAA:303[A]:HOH:O	2.20	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	AAA	100/97 (103%)	94 (94%)	5 (5%)	1 (1%)	15	17
1	BBB	98/97 (101%)	86 (88%)	8 (8%)	4 (4%)	3	1
All	All	198/194 (102%)	180 (91%)	13 (7%)	5 (2%)	9	4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	39[A]	SER
1	BBB	39[B]	SER
1	BBB	38[A]	LEU
1	BBB	38[B]	LEU
1	AAA	53	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	AAA	78/76 (103%)	74 (95%)	4 (5%)	24	33
1	BBB	80/76 (105%)	68 (85%)	12 (15%)	3	3
All	All	158/152 (104%)	142 (90%)	16 (10%)	7	9

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	13	SER

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Mol	Chain	Res	Type
1	AAA	48	LYS
1	AAA	54	ASP
1	AAA	94	LYS
1	BBB	6	SER
1	BBB	8	THR
1	BBB	21[A]	LEU
1	BBB	21[B]	LEU
1	BBB	45	VAL
1	BBB	48	LYS
1	BBB	72	ASN
1	BBB	83	ASN
1	BBB	86	LYS
1	BBB	88	ASN
1	BBB	90	GLU
1	BBB	92	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 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	$\# Z  > 2$
2	ACT	AAA	201	-	1,3,3	4.84	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	201	-	1,3,3	4.14	1 (100%)	0,3,3	0.00	-
5	SO4	AAA	205	3	4,4,4	0.40	0	6,6,6	0.07	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	201	ACT	CH3-C	4.84	1.54	1.48
2	BBB	201	ACT	CH3-C	4.14	1.54	1.48

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
2	AAA	201	ACT	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 [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	AAA	95/97 (97%)	0.02	4 (4%) 36 43	41, 64, 102, 118	0
1	BBB	95/97 (97%)	0.35	10 (10%) 6 8	49, 79, 117, 129	0
All	All	190/194 (97%)	0.18	14 (7%) 14 19	41, 72, 114, 129	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	70	ALA	3.4
1	BBB	16	ALA	3.1
1	BBB	19	ALA	2.8
1	BBB	17	ALA	2.8
1	AAA	16	ALA	2.7
1	AAA	41	ASP	2.7
1	AAA	17[A]	ALA	2.6
1	AAA	70	ALA	2.5
1	BBB	12	ASP	2.5
1	BBB	15	VAL	2.4
1	BBB	69	ALA	2.3
1	BBB	84	THR	2.2
1	BBB	95	VAL	2.1
1	BBB	41	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 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
4	CL	BBB	202	1/1	0.50	0.28	128,128,128,128	0
2	ACT	AAA	201	4/4	0.61	0.34	91,92,96,104	0
2	ACT	BBB	201	4/4	0.75	0.33	116,119,123,124	0
5	SO4	AAA	205	5/5	0.92	0.29	144,144,157,160	0
4	CL	AAA	203	1/1	0.95	0.21	72,72,72,72	0
4	CL	AAA	204	1/1	0.98	0.07	57,57,57,57	0
3	CU	AAA	202	1/1	1.00	0.09	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.