



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7BK6
Title : PfCopC mutant - D83A
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Deposited on : 2021-01-15
Resolution : 2.15 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 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

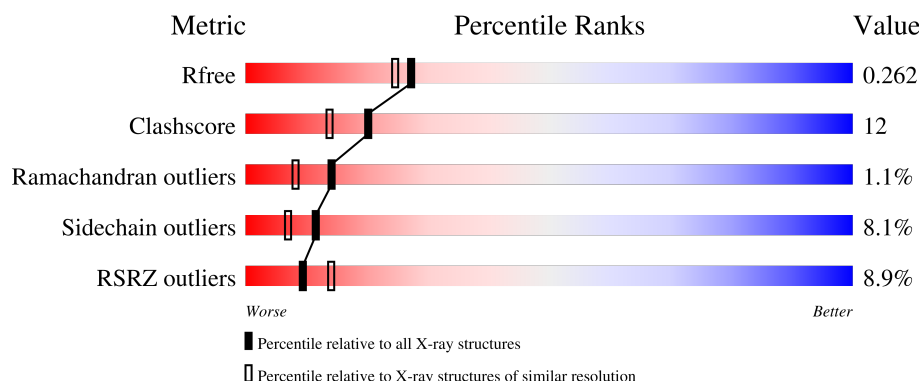
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	AAA	97	<div> <div>8%</div> <div>78%</div> <div>16%</div> <div>.</div> </div>
1	BBB	97	<div> <div>9%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 1529 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	3	0
			719	455	120	144			
1	BBB	96	Total	C	N	O	0	2	0
			710	449	120	141			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

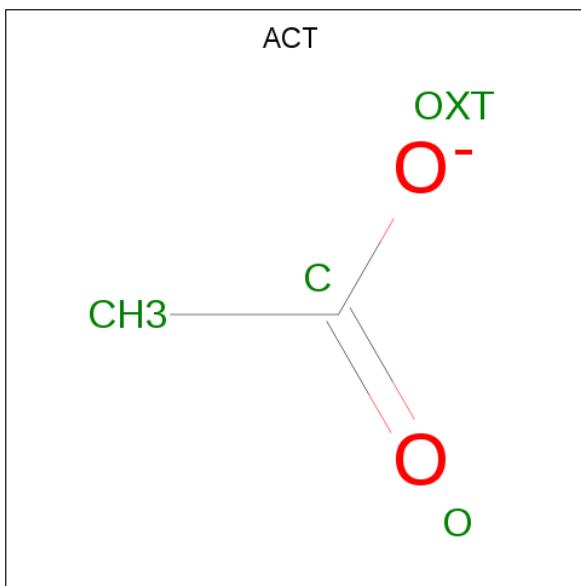
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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


- Molecule 7 is water.

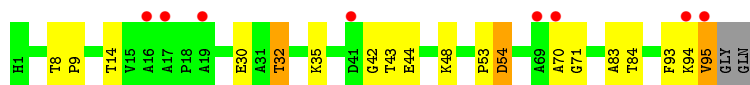
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	58	Total 58	O 58	0	0
7	BBB	29	Total 29	O 29	0	0

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: 



- Molecule 1: Putative copper resistance protein

Chain BBB: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	80.06 Å 80.06 Å 89.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.06 – 2.15 40.03 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.06-2.15) 100.0 (40.03-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.16 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.215 , 0.263 0.221 , 0.262	Depositor DCC
R_{free} test set	787 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.026 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1529	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, CL, CU, NA, ACT

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	0.74	0/732	0.89	0/998
1	BBB	0.65	0/724	0.91	0/988
All	All	0.70	0/1456	0.90	0/1986

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	BBB	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	89	GLY	Peptide

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	AAA	719	0	723	20	0
1	BBB	710	0	715	22	0
2	AAA	1	0	0	0	0
3	AAA	1	0	0	0	0
4	AAA	2	0	0	1	0
5	AAA	5	0	0	0	0
6	BBB	4	0	3	0	0
7	AAA	58	0	0	5	1
7	BBB	29	0	0	8	1
All	All	1529	0	1441	36	1

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 (36) 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:AAA:83:ALA:HB2	7:AAA:248:HOH:O	1.49	1.10
1:BBB:23:LEU:HD12	7:BBB:308:HOH:O	1.71	0.89
1:AAA:30[B]:GLU:OE1	7:AAA:201:HOH:O	1.92	0.87
1:BBB:21:LEU:CB	7:BBB:308:HOH:O	2.23	0.85
1:BBB:21:LEU:HB2	7:BBB:308:HOH:O	1.79	0.80
1:AAA:83:ALA:O	1:AAA:84:THR:HB	1.86	0.75
1:BBB:54:ASP:OD1	7:BBB:301:HOH:O	2.12	0.68
1:BBB:10[A]:ALA:O	1:BBB:11[A]:ALA:CB	2.45	0.65
1:BBB:75:VAL:O	1:BBB:90:GLU:O	2.14	0.63
1:AAA:42:GLY:HA2	7:AAA:238:HOH:O	2.00	0.61
1:AAA:8:THR:HA	1:AAA:9:PRO:C	2.23	0.59
1:BBB:21:LEU:C	7:BBB:308:HOH:O	2.40	0.58
1:AAA:32[A]:THR:HG21	1:BBB:47:ILE:CD1	2.34	0.57
1:AAA:30[B]:GLU:CD	7:AAA:201:HOH:O	2.39	0.56
1:AAA:70:ALA:HA	1:AAA:95[B]:VAL:HG22	1.88	0.54
1:BBB:10[A]:ALA:O	1:BBB:11[A]:ALA:HB3	2.08	0.52
1:BBB:22:ARG:N	7:BBB:308:HOH:O	2.44	0.51
1:BBB:23:LEU:CD1	7:BBB:308:HOH:O	2.41	0.50
1:BBB:10[B]:ALA:O	1:BBB:13:SER:OG	2.26	0.50
1:AAA:44:GLU:OE2	4:AAA:104:CL:CL	2.67	0.49
1:AAA:32[A]:THR:HG21	1:BBB:47:ILE:HD12	1.94	0.49
1:AAA:93:PHE:O	7:AAA:202:HOH:O	2.20	0.48
1:BBB:7:ALA:O	1:BBB:10[A]:ALA:HA	2.14	0.48
1:BBB:21:LEU:HB3	7:BBB:308:HOH:O	2.04	0.48
1:AAA:32[A]:THR:HG23	1:BBB:47:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:16:ALA:O	1:BBB:18:PRO:HD3	2.15	0.47
1:AAA:70:ALA:HA	1:AAA:95[A]:VAL:HG22	1.98	0.46
1:AAA:35:LYS:HA	1:BBB:32:THR:O	2.16	0.45
1:BBB:34:THR:HG23	1:BBB:79:ALA:HA	1.99	0.43
1:AAA:14:THR:HA	1:AAA:94:LYS:O	2.20	0.42
1:AAA:71:GLY:O	1:AAA:94:LYS:HA	2.18	0.42
1:BBB:24:THR:HA	1:BBB:58:LYS:O	2.20	0.42
1:AAA:8:THR:CA	1:AAA:9:PRO:C	2.88	0.41
1:AAA:54:ASP:OD1	1:AAA:54:ASP:N	2.54	0.41
1:AAA:32[A]:THR:HG23	1:BBB:47:ILE:HG21	2.01	0.41
1:AAA:32[A]:THR:CG2	1:BBB:47:ILE:HG21	2.52	0.40

All (1) 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)
7:AAA:248:HOH:O	7:BBB:323:HOH:O[4_454]	2.16	0.04

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	95/97 (98%)	90 (95%)	4 (4%)	1 (1%)	14	8
1	BBB	96/97 (99%)	84 (88%)	11 (12%)	1 (1%)	15	9
All	All	191/194 (98%)	174 (91%)	15 (8%)	2 (1%)	14	9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	84	THR
1	AAA	53	PRO

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	AAA	77/75 (103%)	70 (91%)	7 (9%)	9	5
1	BBB	74/75 (99%)	67 (90%)	7 (10%)	8	4
All	All	151/150 (101%)	137 (91%)	14 (9%)	11	5

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	32[A]	THR
1	AAA	32[B]	THR
1	AAA	43	THR
1	AAA	48	LYS
1	AAA	54	ASP
1	AAA	95[A]	VAL
1	AAA	95[B]	VAL
1	BBB	39	SER
1	BBB	45	VAL
1	BBB	48	LYS
1	BBB	51	GLU
1	BBB	78	ASN
1	BBB	91	TYR
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 [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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
5	SO4	AAA	105	2	4,4,4	0.34	0	6,6,6	0.14	0
6	ACT	BBB	201	-	1,3,3	4.00	1 (100%)	0,3,3	0.00	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	BBB	201	ACT	CH3-C	4.00	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	AAA	95/97 (97%)	0.62	8 (8%)	11 15	44, 64, 96, 110	0
1	BBB	96/97 (98%)	0.67	9 (9%)	8 12	49, 75, 102, 114	0
All	All	191/194 (98%)	0.64	17 (8%)	9 14	44, 71, 101, 114	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	96	GLY	4.9
1	AAA	17	ALA	4.8
1	BBB	68	LEU	3.8
1	AAA	69	ALA	3.7
1	AAA	95[A]	VAL	3.1
1	BBB	95	VAL	2.9
1	AAA	41	ASP	2.9
1	BBB	69	ALA	2.9
1	BBB	70	ALA	2.8
1	AAA	16	ALA	2.7
1	AAA	70	ALA	2.6
1	BBB	41	ASP	2.5
1	BBB	16	ALA	2.5
1	BBB	72	ASN	2.5
1	AAA	19	ALA	2.4
1	BBB	94	LYS	2.3
1	AAA	94	LYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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(Å ²)	Q<0.9
6	ACT	BBB	201	4/4	0.71	0.37	107,109,109,116	0
5	SO4	AAA	105	5/5	0.92	0.17	95,99,110,117	0
3	NA	AAA	102	1/1	0.92	0.09	56,56,56,56	0
4	CL	AAA	103	1/1	0.96	0.24	59,59,59,59	0
4	CL	AAA	104	1/1	0.98	0.15	90,90,90,90	0
2	CU	AAA	101	1/1	1.00	0.14	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.