



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:04 PM UTC

PDB ID : 4DNR / pdb\_00004dnr  
Title : Crystal structure of the CusBA heavy-metal efflux complex from Escherichia coli, E716F mutant  
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Deposited on : 2012-02-08  
Resolution : 3.68 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0  
Xtrriage (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

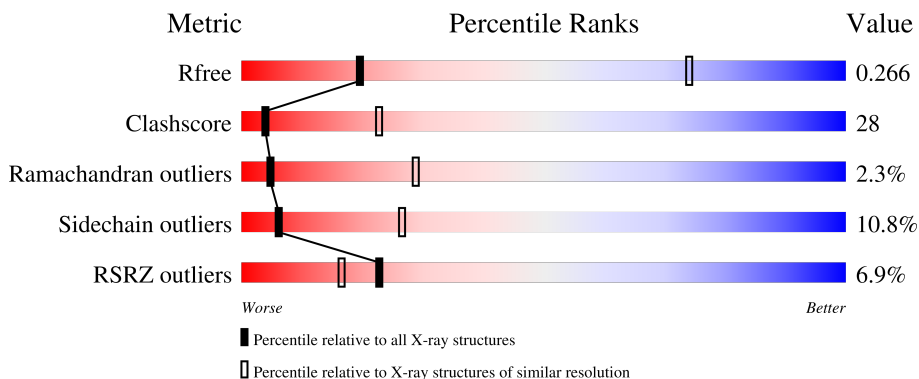
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.68 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	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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	413	
1	C	413	
2	A	1054	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12887 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 Cation efflux system protein CusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
1	C	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	expression tag	UNP P77239
B	409	HIS	-	expression tag	UNP P77239
B	410	HIS	-	expression tag	UNP P77239
B	411	HIS	-	expression tag	UNP P77239
B	412	HIS	-	expression tag	UNP P77239
B	413	HIS	-	expression tag	UNP P77239
C	408	HIS	-	expression tag	UNP P77239
C	409	HIS	-	expression tag	UNP P77239
C	410	HIS	-	expression tag	UNP P77239
C	411	HIS	-	expression tag	UNP P77239
C	412	HIS	-	expression tag	UNP P77239
C	413	HIS	-	expression tag	UNP P77239

- Molecule 2 is a protein called Cation efflux system protein CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	1031	Total	C	N	O	S	0	0	0
			7950	5144	1333	1436	37			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P38054
A	-5	HIS	-	expression tag	UNP P38054

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP P38054
A	-3	HIS	-	expression tag	UNP P38054
A	-2	HIS	-	expression tag	UNP P38054
A	-1	HIS	-	expression tag	UNP P38054
A	0	HIS	-	expression tag	UNP P38054
A	716	PHE	GLU	engineered mutation	UNP P38054

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

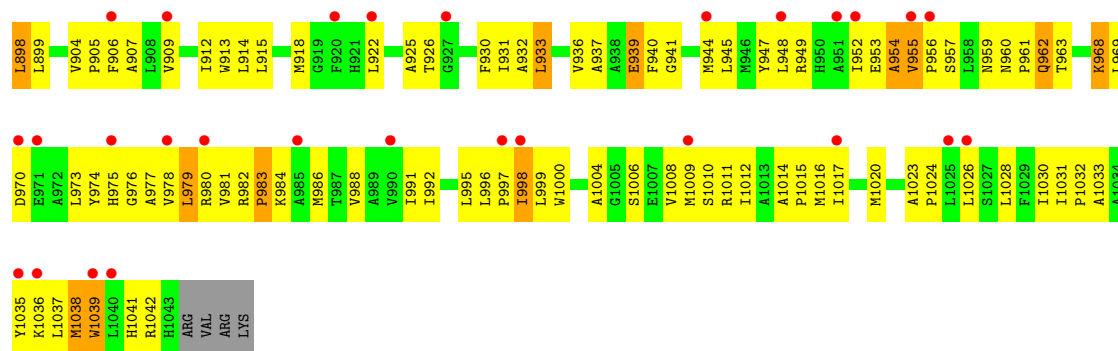
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0

- Molecule 4 is water.

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







## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.59Å 159.59Å 689.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.67 – 3.68 97.67 – 3.68	Depositor EDS
% Data completeness (in resolution range)	89.9 (97.67-3.68) 98.8 (97.67-3.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.67Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.244 , 0.272 0.238 , 0.266	Depositor DCC
$R_{free}$ test set	1872 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.3	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 111.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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:  
CU

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	0.27	0/2498	0.74	2/3401 (0.1%)
1	C	0.27	0/2513	0.74	0/3421
2	A	0.29	0/8117	0.76	6/11052 (0.1%)
All	All	0.28	0/13128	0.75	8/17874 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	562	LEU	CA-C-N	-7.41	110.57	119.84
2	A	562	LEU	C-N-CA	-7.41	110.57	119.84
2	A	535	TRP	CA-C-N	5.52	124.71	118.97
2	A	535	TRP	C-N-CA	5.52	124.71	118.97
2	A	473	ARG	N-CA-C	-5.42	106.62	113.18

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	B	2458	0	2522	118	0
1	C	2473	0	2533	103	0
2	A	7950	0	8198	534	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	C	4	0	0	0	0
All	All	12887	0	13253	735	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 28.

The worst 5 of 735 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:385:ILE:HG22	1:B:389:ALA:HB2	1.36	1.06
2:A:327:ARG:HH11	2:A:666:ILE:HG13	1.27	0.95
2:A:395:GLY:HA3	2:A:478:LEU:HB3	1.49	0.93
2:A:51:THR:HG22	2:A:127:ALA:HA	1.49	0.90
2:A:955:VAL:HG13	2:A:956:PRO:HD3	1.55	0.88

There are no symmetry-related clashes.

## 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	B	320/413 (78%)	280 (88%)	33 (10%)	7 (2%)	5	29
1	C	322/413 (78%)	294 (91%)	25 (8%)	3 (1%)	14	45
2	A	1027/1054 (97%)	891 (87%)	107 (10%)	29 (3%)	4	26
All	All	1669/1880 (89%)	1465 (88%)	165 (10%)	39 (2%)	5	29

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	ASP
1	B	390	ASN
2	A	123	ALA
2	A	138	TRP
2	A	293	SER

### 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	263/338 (78%)	243 (92%)	20 (8%)	12	38
1	C	265/338 (78%)	242 (91%)	23 (9%)	9	33
2	A	850/872 (98%)	744 (88%)	106 (12%)	4	21
All	All	1378/1548 (89%)	1229 (89%)	149 (11%)	6	26

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	694	ASP
2	A	979	LEU
2	A	722	ARG
2	A	848	VAL
2	A	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	518	ASN
2	A	769	ASN
2	A	526	HIS
2	A	635	GLN
2	A	861	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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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 [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	322/413 (77%)	-0.02	2 (0%) 85 65	21, 61, 104, 218	0
1	C	324/413 (78%)	-0.04	1 (0%) 90 76	27, 62, 105, 170	0
2	A	1031/1054 (97%)	0.66	112 (10%) 10 11	20, 103, 216, 505	0
All	All	1677/1880 (89%)	0.40	115 (6%) 23 16	20, 74, 202, 505	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	715	ALA	4.9
2	A	717	ARG	4.9
2	A	1036	LYS	4.6
2	A	980	ARG	4.3
2	A	563	PRO	4.3

### 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	CU	A	1101	1/1	0.99	0.04	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.