

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 4, 2024 - 06:17 pm BST

PDB ID	:	6GT0
Title	:	Nitrite-bound copper nitrite reductase from Achromobacter cycloclastes deter-
		mined by serial femtosecond rotation crystallography
Authors	:	Halsted, T.P.; Yamashita, K.; Gopalasingam, C.C.; Shenoy, R.T.; Hirata, K.;
		Ago, H.; Ueno, G.; Eady, R.R.; Antonyuk, S.V.; Yamamoto, M.; Hasnain, S.S.
Deposited on	:	2018-06-15
Resolution	:	1.50  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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

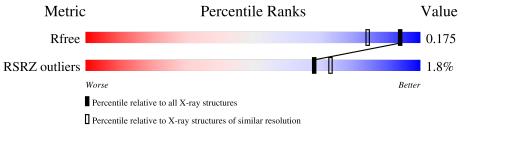
MolProbity Mogul		FAILED 1.8.4, CSD as541be (2020)
Xtriage (Phenix)		
$\mathrm{EDS}$	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	2936 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



#### $6 \mathrm{GT0}$

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3047 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.

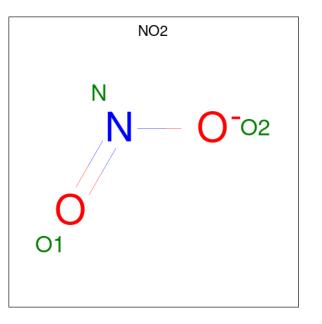
• Molecule 1 is a protein called Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	333	Total 2595	C 1654	N 441	O 490	S 10	0	4	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Cu 2 2	0	0

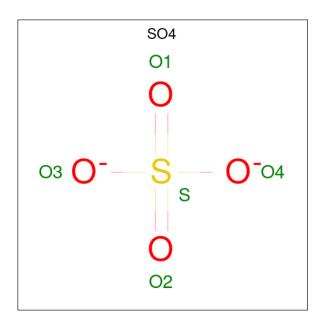
• Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 6	N 2	0 4	0	1

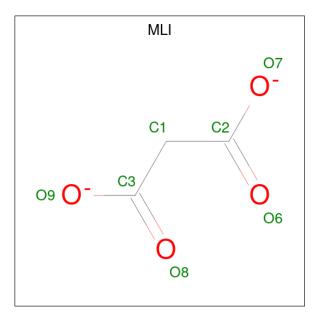
• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





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

• Molecule 5 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  3  4 \end{array}$	0	0



• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	395	Total         O           418         418	0	39

MolProbity failed to run properly - this section is therefore empty.



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants	94.92Å 94.92Å 94.92Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	54.86 - 1.50	Depositor
Resolution (A)	54.80 - 1.50	EDS
% Data completeness	100.0 (54.86 - 1.50)	Depositor
(in resolution range)	100.0 (54.80-1.50)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.17 (at 1.50 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
$R, R_{free}$	0.143 , $0.171$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.151 , $0.175$	DCC
$R_{free}$ test set	2295 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	18.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, $48.8$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.042 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3047	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 4 Model quality (i)

### 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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



Mal	Trune	Chain	Res	Link	B	ond leng	$\operatorname{gths}$	B	ond ang	gles
Mol	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NO2	А	503[A]	2	$1,\!2,\!2$	0.20	0	0,1,1	-	-
3	NO2	А	503[B]	2	$1,\!2,\!2$	0.55	0	$0,\!1,\!1$	-	-
5	MLI	А	505	-	$6,\!6,\!6$	0.98	0	7,7,7	1.30	1 (14%)
5	MLI	А	507	-	$6,\!6,\!6$	1.27	0	7,7,7	0.76	0
5	MLI	А	506	-	$6,\!6,\!6$	1.32	1 (16%)	7,7,7	0.89	0
4	SO4	А	504	-	$4,\!4,\!4$	0.35	0	$6,\!6,\!6$	0.91	0

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).

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
5	MLI	А	507	-	-	2/4/4/4	-
5	MLI	А	506	-	-	0/4/4/4	-
5	MLI	А	505	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	506	MLI	O9-C3	-2.37	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	505	MLI	O6-C2-C1	-2.26	115.48	122.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	507	MLI	C2-C1-C3-O8
5	А	507	MLI	C2-C1-C3-O9
5	А	505	MLI	C2-C1-C3-O9

There are no ring outliers.

No monomer is involved in short contacts.



## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 5 Fit of model and data (i)

## 5.1 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,  $95^{th}$  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			$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9		
1	А	333/378~(88%)	-0.10	6 (1%)	68	73	14, 17, 28, 58	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	340	MET	4.2
1	А	199	PRO	2.9
1	А	196	TYR	2.8
1	А	200	GLY	2.7
1	А	11	THR	2.1

#### 5.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.4 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	MLI	А	507	7/7	0.84	0.19	23,41,59,60	0
4	SO4	А	504	5/5	0.85	0.14	32,42,44,45	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NO2	А	503[A]	3/3	0.87	0.28	$15,\!15,\!18,\!20$	3
3	NO2	А	503[B]	3/3	0.87	0.28	16,16,19,20	3
5	MLI	А	506	7/7	0.89	0.16	26,31,32,33	0
5	MLI	А	505	7/7	0.90	0.18	26,33,36,36	0
2	CU	А	502	1/1	0.99	0.03	16,16,16,16	0
2	CU	А	501	1/1	1.00	0.04	16,16,16,16	0

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## 5.5 Other polymers (i)

There are no such residues in this entry.

