



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:52 PM GMT

PDB ID : 1NIB  
Title : THE STRUCTURE OF CU-NITRITE REDUCTASE FROM ACHROMOBACTER CYCLOCLASTES AT FIVE PH VALUES, WITH NITRITE BOUND AND WITH TYPE II CU DEPLETED  
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Deposited on : 1995-07-03  
Resolution : 2.70 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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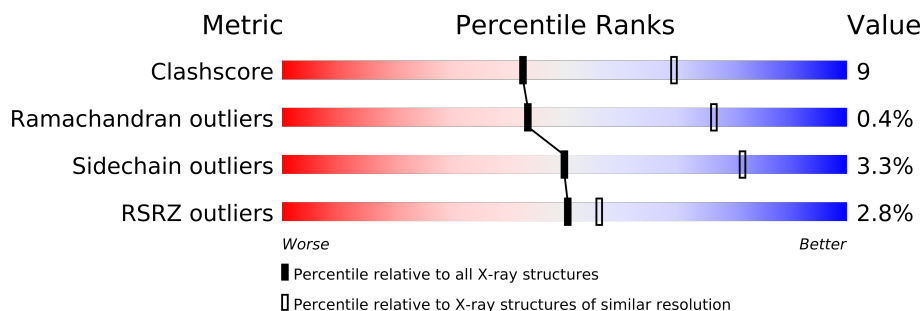
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	
1	C	340	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8290 atoms, of which 84 are hydrogens and 0 are deuterium.

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 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	H	N	O	S	0	0	0
			2587	1632	28	439	478	10			
1	B	333	Total	C	H	N	O	S	0	0	0
			2583	1630	28	439	476	10			
1	C	333	Total	C	H	N	O	S	0	0	0
			2583	1630	28	439	476	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		
2	C	2	Total	Cu	0	0
			2	2		

- Molecule 3 is water.

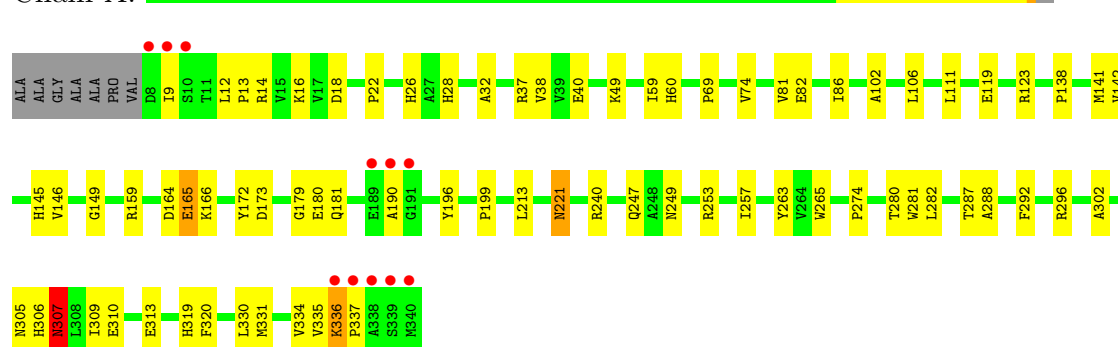
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	1	0
			178	178		
3	B	176	Total	O	2	0
			176	176		
3	C	177	Total	O	6	0
			177	177		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

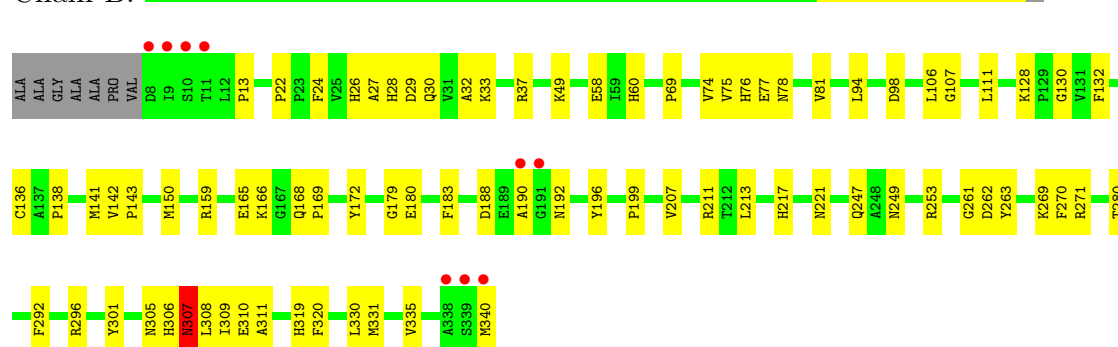
#### • Molecule 1: NITRITE REDUCTASE

Chain A:



#### • Molecule 1: NITRITE REDUCTASE

Chain B:



#### • Molecule 1: NITRITE REDUCTASE

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.56Å 115.36Å 115.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 49.78 – 2.57	Depositor EDS
% Data completeness (in resolution range)	85.0 (10.00-2.70) 70.7 (49.78-2.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.39 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.155 , (Not available) 0.172 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.5	EDS
Estimated twinning fraction	0.036 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 30551 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	A	0.45	0/2629	0.78	4/3586 (0.1%)
1	B	0.46	0/2625	0.77	2/3580 (0.1%)
1	C	0.50	1/2625 (0.0%)	0.79	1/3580 (0.0%)
All	All	0.47	1/7879 (0.0%)	0.78	7/10746 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	165	GLU	CD-OE2	7.54	1.33	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	GLU	OE1-CD-OE2	-7.89	113.84	123.30
1	C	307	ASN	N-CA-C	-7.26	91.39	111.00
1	A	307	ASN	N-CA-C	-6.60	93.17	111.00
1	B	307	ASN	N-CA-C	-6.35	93.85	111.00
1	A	282	LEU	CA-CB-CG	5.57	128.11	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2559	28	2449	49	8
1	B	2555	28	2446	59	5
1	C	2555	28	2446	41	13
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	178	0	0	8	9
3	B	176	0	0	14	6
3	C	177	0	0	9	9
All	All	8206	84	7341	135	25

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 135 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:32:ALA:HA	3:B:573:HOH:O	1.43	1.15
1:A:13:PRO:HG2	1:A:37:ARG:HG2	1.54	0.90
1:B:165:GLU:OE1	3:B:615:HOH:O	1.92	0.88
1:A:32:ALA:HA	3:A:574:HOH:O	1.76	0.85
1:A:336:LYS:HE2	3:C:4393:HOH:O	1.75	0.84

The worst 5 of 25 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	Distance(Å)	Clash(Å)
1:C:119:GLU:O	3:A:654:HOH:O[4_555]	1.19	1.01
1:B:29:ASP:OD2	1:C:8:ASP:N[2_565]	1.21	0.99
1:A:14:ARG:NE	3:A:656:HOH:O[4_455]	1.31	0.89
1:A:18:ASP:CB	3:C:4455:HOH:O[4_455]	1.31	0.89
1:C:119:GLU:C	3:A:654:HOH:O[4_555]	1.36	0.84

## 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	A	331/340 (97%)	318 (96%)	11 (3%)	2 (1%)	33	66
1	B	331/340 (97%)	320 (97%)	10 (3%)	1 (0%)	50	82
1	C	331/340 (97%)	320 (97%)	10 (3%)	1 (0%)	50	82
All	All	993/1020 (97%)	958 (96%)	31 (3%)	4 (0%)	43	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	HIS
1	A	336	LYS
1	B	306	HIS
1	C	306	HIS

### 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	A	266/273 (97%)	258 (97%)	8 (3%)	53	84
1	B	265/273 (97%)	257 (97%)	8 (3%)	53	84
1	C	265/273 (97%)	255 (96%)	10 (4%)	44	76
All	All	796/819 (97%)	770 (97%)	26 (3%)	50	81

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	141	MET
1	B	307	ASN
1	C	320	PHE
1	B	213	LEU
1	B	253	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	HIS

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Mol	Chain	Res	Type
1	B	76	HIS
1	C	28	HIS
1	B	26	HIS
1	B	28	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are 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.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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, 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	A	333/340 (97%)	-0.69	11 (3%)	44 49	2, 6, 23, 55	4 (1%)
1	B	333/340 (97%)	-0.58	9 (2%)	52 57	2, 6, 27, 46	4 (1%)
1	C	333/340 (97%)	-0.67	8 (2%)	56 62	2, 5, 27, 54	4 (1%)
All	All	999/1020 (97%)	-0.65	28 (2%)	50 56	2, 6, 27, 55	12 (1%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	ALA	15.6
1	A	339	SER	10.9
1	B	340	MET	8.3
1	A	340	MET	8.0
1	B	8	ASP	7.1

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	B	502	1/1	0.04	-2.56	8,8,8,8	0
2	CU	A	501	1/1	0.03	-3.44	8,8,8,8	0
2	CU	B	501	1/1	0.04	-4.37	11,11,11,11	0
2	CU	C	502	1/1	0.04	-6.04	5,5,5,5	0
2	CU	A	502	1/1	0.05	-6.65	13,13,13,13	0
2	CU	C	501	1/1	0.03	-7.38	12,12,12,12	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.