

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

Aug 30, 2023 – 01:38 pm BST

PDB ID	:	8C46
Title	:	N-Carbamoyl-beta-Alanine Amidohydrolases from Rhizobium radiobacter
		MDC 8606
Authors	:	Basle, A.; Marles-Wright, J.
Deposited on	:	2023-01-02
Resolution	:	2.00  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 (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:

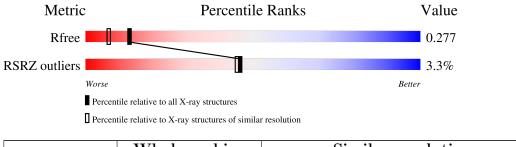
MolProbity	:	FAILED
		1.8.4, CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35
buster-report	:	1.1.7 (2018)
-		20191225.v01 (using entries in the PDB archive December 25th 2019)
		5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)		Engh & Huber (2001)
Ideal geometry (DNA, RNA)		3
Validation Pipeline (wwPDB-VP)	:	2.35

# 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 2.00 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 $(\#Entries)$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	8085 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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



# 2 Entry composition (i)

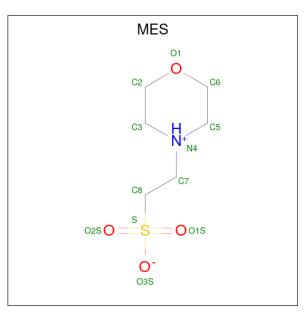
There are 4 unique types of molecules in this entry. The entry contains 12364 atoms, of which 5778 are hydrogens and 0 are deuteriums.

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 N-carbamoyl-beta-alanine amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	А	409	Total 5974	C 1942	Н 2876	N 547	O 589	S 20	0	0	0
1	В	409	Total 5974	C 1942			O 589	S 20	0	0	0

• Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
0	2 A	1	Total	С	Η	Ν	0	S	0	0	
			25	6	13	1	4	1			
0	р	1	Total	С	Η	Ν	0	S	0	0	
	В	1	25	6	13	1	4	1		0	

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Zn 2 2	0	0
3	В	2	Total Zn 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	179	Total O 179 179	0	0
4	В	183	Total O 183 183	0	0

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



## 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	53.23Å 104.62Å 145.37Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	84.92 - 2.00	Depositor
Resolution (A)	84.92 - 2.00	EDS
% Data completeness	99.8 (84.92-2.00)	Depositor
(in resolution range)	99.8 (84.92-2.00)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.96 (at 2.00 \text{\AA})$	Xtriage
Refinement program	BUSTER, REFMAC 5	Depositor
D D.	0.229 , $0.270$	Depositor
$R, R_{free}$	0.236 , $0.277$	DCC
$R_{free}$ test set	2802 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	23.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.41 , $47.9$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.52, \langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12364	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 40.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7344e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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 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



101102												
Mal	Mol Type	Chain	Res	Link		ond leng		Bond angles				
IVIOI					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
2	MES	В	501	-	12,12,12	0.65	0	14,16,16	1.83	2 (14%)		
2	MES	А	501	-	12,12,12	0.94	0	14,16,16	0.62	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
2	MES	В	501	-	-	0/6/14/14	0/1/1/1
2	MES	А	501	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	501	MES	O1S-S-C8	-4.70	101.26	106.92
2	В	501	MES	O3S-S-C8	4.19	112.54	105.77

There are no chirality outliers.

There are no torsion outliers.

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	409/409~(100%)	0.35	15 (3%) 41 41	15, 28, 57, 73	0
1	В	409/409 (100%)	0.32	12 (2%) 51 50	17, 27, 55, 78	0
All	All	818/818 (100%)	0.33	27 (3%) 46 45	15, 27, 57, 78	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	28	ILE	7.8	
1	А	28	ILE	5.0	
1	А	29	ALA	3.7	
1	В	165	THR	3.6	
1	А	156	TYR	3.4	
1	В	163	GLY	3.4	
1	А	30	GLY	3.2	
1	А	174	GLY	3.1	
1	В	156	TYR	2.7	
1	В	171	LYS	2.7	
1	А	26	PRO	2.6	
1	В	47	LEU	2.5	
1	А	176	LEU	2.4	
1	А	93	GLY	2.4	
1	А	381	ASP	2.4	
1	А	50	ARG	2.2	
1	А	175	TRP	2.2	
1	В	168	GLU	2.2	
1	А	43	GLU	2.2	
1	В	176	LEU	2.1	
1	А	165	THR	2.1	
1	В	177	GLY	2.1	
1	В	161	THR	2.1	
1	B	162	ASP	2.1	

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Mol	Chain	Res	Type	RSRZ
1	В	413	ILE	2.1
1	А	149	ILE	2.0
1	А	382	GLY	2.0

### 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.

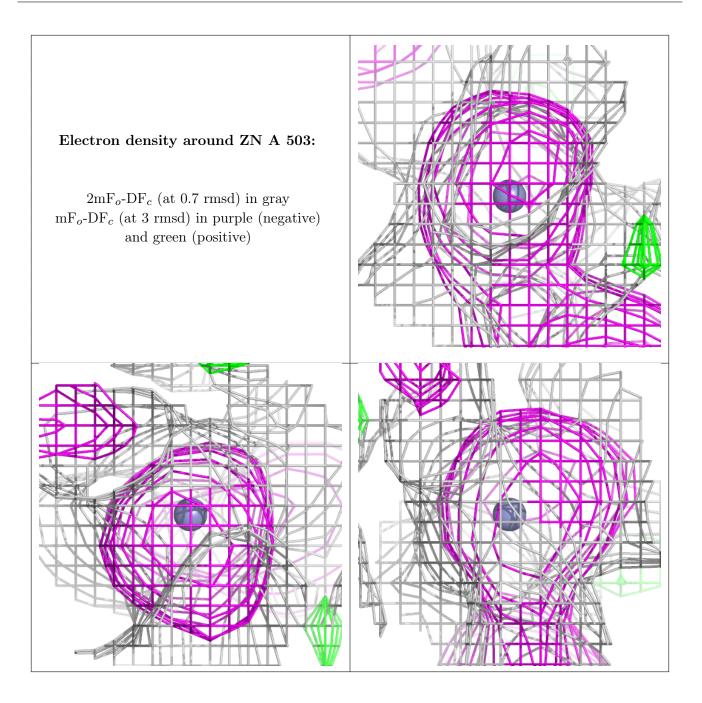
### 5.4 Ligands (i)

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.

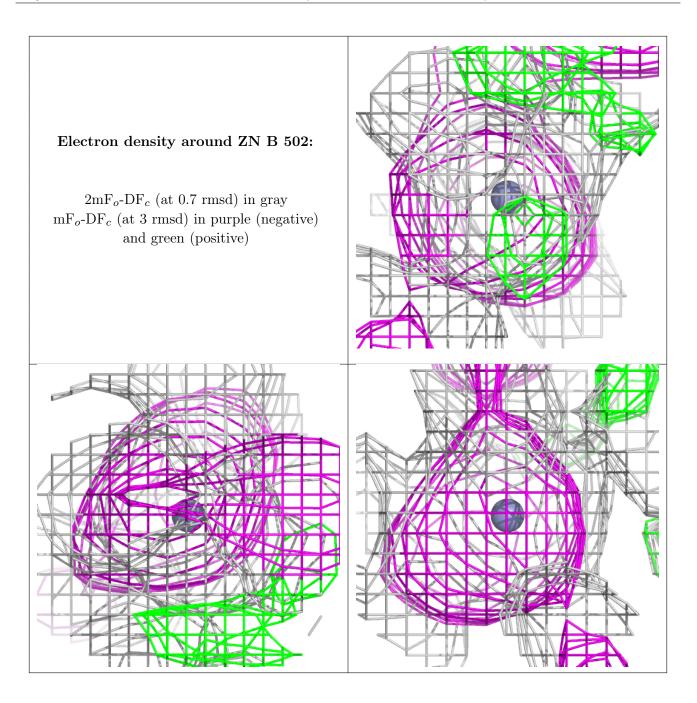
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	ZN	А	503	1/1	0.93	0.07	40,40,40,40	0
2	MES	В	501	12/12	0.94	0.15	28,31,34,36	0
2	MES	А	501	12/12	0.95	0.17	22,34,47,48	0
3	ZN	В	502	1/1	0.97	0.07	$38,\!38,\!38,\!38$	0
3	ZN	В	503	1/1	0.99	0.09	30,30,30,30	0
3	ZN	А	502	1/1	1.00	0.05	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

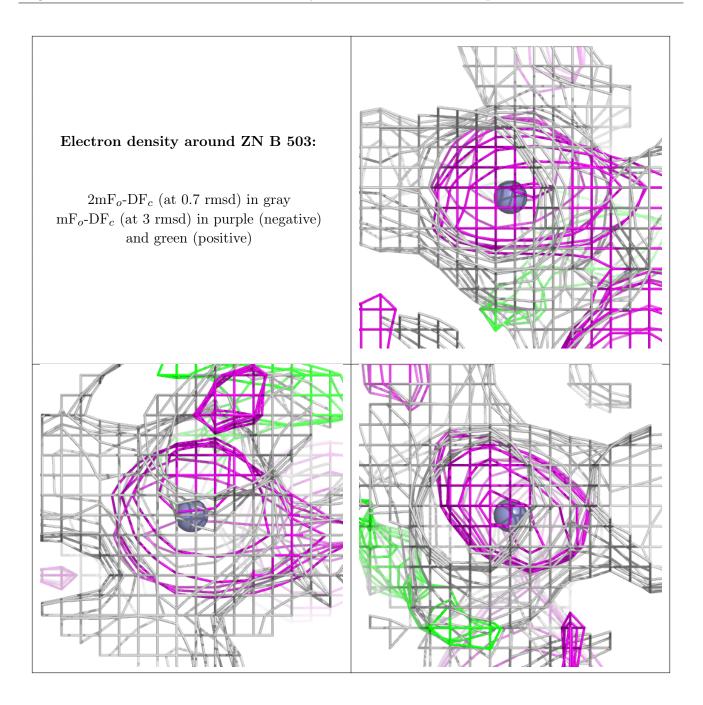




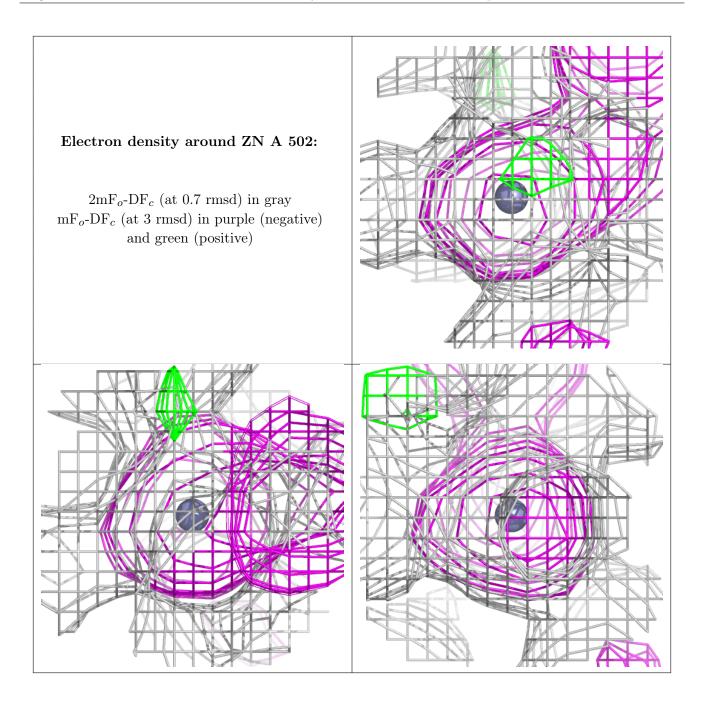












### 5.5 Other polymers (i)

There are no such residues in this entry.

