

# Full wwPDB Geometry-Only Validation Report (i)

#### Sep 13, 2023 – 05:17 PM EDT

PDB ID : 4Q49

Title : Room temperature neutron crystal structure of apo human carbonic anhydrase

at pH 7.5

Authors: Fisher, S.Z.; McKenna, R.

Deposited on : 2014-04-14

Resolution : 1.80 Å(reported)

This is a Full wwPDB Geometry-Only 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

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $NEUTRON\ DIFFRACTION$ 

The reported resolution of this entry is 1.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4639 atoms, of which 1563 are hydrogens and 828 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 Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace		
1	А	258	Total	С	D	Н	N	О	S	76	0	0
1	11		4074	1321	452	1563	355	381	2	'0	0	

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

$\mathbf{Mol}$	Chain Residues		Atoms	ZeroOcc	AltConf	
2	A	1	Total Zn 1 1	0	0	

• Molecule 3 is water.

Mol	Chain	Residues	A	toms		ZeroOcc	AltConf
3	A	188	Total 564	D 376	O 188	0	0

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.



## 3 Model quality (i)

### 3.1 Standard geometry (i)

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

### 3.2 Too-close contacts (i)

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

### 3.3 Torsion angles (i)

#### 3.3.1 Protein backbone (i)

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

#### 3.3.2 Protein sidechains (i)

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

#### 3.3.3 RNA (i)

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

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

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

### 3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 3.6 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.

## 3.7 Other polymers (i)

There are no such residues in this entry.

## 3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

