



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:21 am BST

PDB ID : 1YDD  
Title : STRUCTURAL BASIS OF INHIBITOR AFFINITY TO VARIANTS OF HUMAN CARBONIC ANHYDRASE II  
Authors : Nair, S.K.; Christianson, D.W.  
Deposited on : 1994-12-22  
Resolution : 2.10 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](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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.11

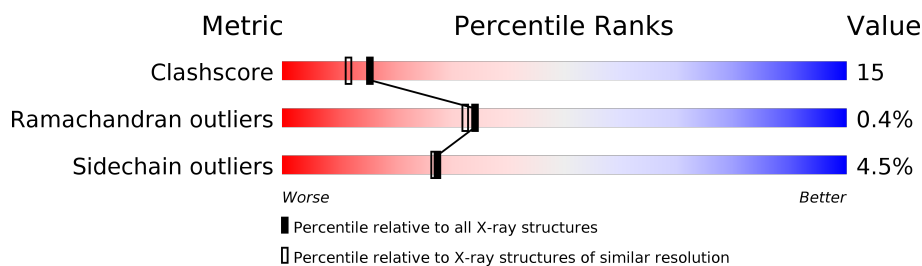
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2158 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 CARBONIC ANHYDRASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2042	1309	353	378	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ARG	LEU	CONFLICT	UNP P00918

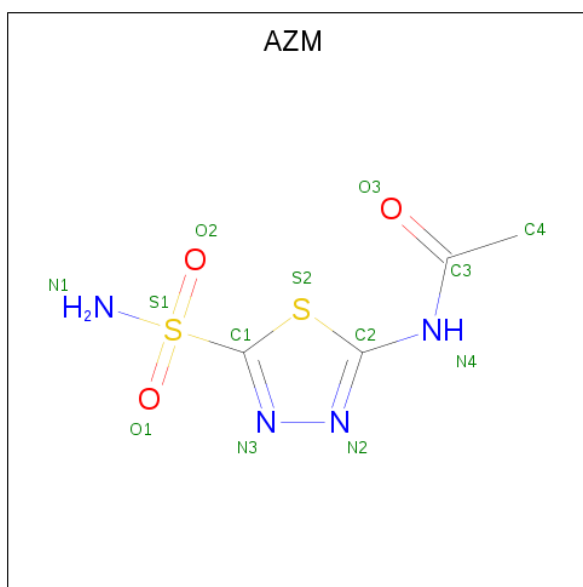
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 4 is 5-ACETAMIDO-1,3,4-THIADIAZOLE-2-SULFONAMIDE (three-letter code: AZM) (formula: C<sub>4</sub>H<sub>6</sub>N<sub>4</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	4	4	3	2		

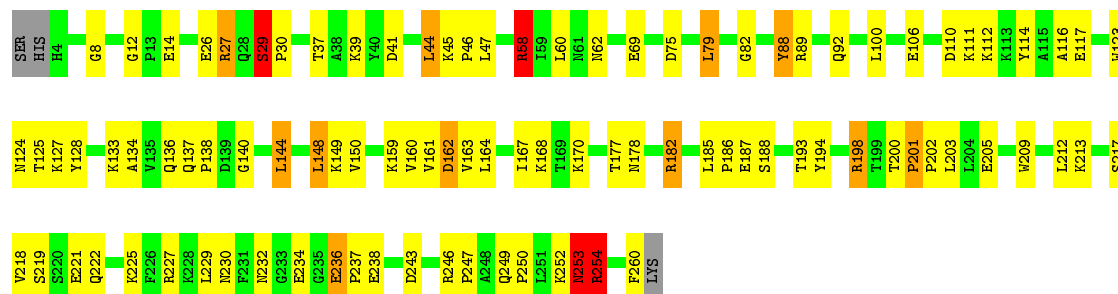
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		



Note EDS was not executed.

Chain A:  61% 32% . .



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.70 Å   41.70 Å   73.00 Å 90.00°   104.60°   90.00°	Depositor
Resolution (Å)	6.50 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (6.50-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

## 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: ZN, AZM, HG

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	1.44	11/2102 (0.5%)	1.61	27/2851 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLU	CD-OE2	8.24	1.34	1.25
1	A	117	GLU	CD-OE2	7.65	1.34	1.25
1	A	26	GLU	CD-OE2	7.54	1.33	1.25
1	A	234	GLU	CD-OE1	6.68	1.32	1.25
1	A	188	SER	CB-OG	6.43	1.50	1.42
1	A	221	GLU	CD-OE1	6.23	1.32	1.25
1	A	29	SER	CB-OG	-5.98	1.34	1.42
1	A	14	GLU	CD-OE1	5.79	1.32	1.25
1	A	106	GLU	CD-OE1	-5.77	1.19	1.25
1	A	236	GLU	CD-OE2	5.69	1.31	1.25
1	A	187	GLU	CD-OE1	5.62	1.31	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ARG	NE-CZ-NH1	13.77	127.18	120.30
1	A	29	SER	CA-C-O	-9.70	99.73	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	SER	O-C-N	9.26	138.70	121.10
1	A	58	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	A	201	PRO	CA-C-O	-8.90	98.83	120.20
1	A	58	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	254	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	202	PRO	N-CA-CB	8.00	112.90	103.30
1	A	202	PRO	CA-N-CD	-7.96	100.36	111.50
1	A	27	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	227	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	30	PRO	CA-N-CD	-7.57	100.90	111.50
1	A	202	PRO	N-CD-CG	7.32	114.17	103.20
1	A	30	PRO	N-CA-CB	7.23	111.98	103.30
1	A	162	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	88	TYR	CB-CG-CD2	-6.54	117.07	121.00
1	A	182	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	182	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	201	PRO	O-C-N	6.32	133.11	121.10
1	A	148	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	243	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	30	PRO	N-CD-CG	6.10	112.35	103.20
1	A	106	GLU	CG-CD-OE1	5.95	130.20	118.30
1	A	198	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	75	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	162	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	89	ARG	NE-CZ-NH1	5.37	122.98	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain
1	A	254	ARG	Sidechain
1	A	58	ARG	Sidechain

## 5.2 Too-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 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	A	2042	0	1989	59	2
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	13	0	5	1	0
5	A	101	0	0	4	0
All	All	2158	0	1994	60	2

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 15.

All (60) 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:A:125:THR:C	1:A:127:LYS:N	2.20	0.94
1:A:253:ASN:HD22	1:A:254:ARG:N	1.70	0.87
1:A:198:ARG:HG2	1:A:200:THR:H	1.47	0.78
1:A:253:ASN:ND2	1:A:254:ARG:N	2.35	0.74
1:A:198:ARG:HD2	1:A:200:THR:O	1.92	0.69
1:A:159:LYS:HB2	5:A:343:HOH:O	1.94	0.67
1:A:253:ASN:HD22	1:A:253:ASN:C	1.99	0.64
4:A:264:AZM:S2	4:A:264:AZM:O3	2.56	0.64
1:A:110:ASP:O	1:A:111:LYS:HB2	1.97	0.64
1:A:198:ARG:CD	1:A:200:THR:O	2.47	0.62
1:A:58:ARG:NH1	1:A:60:LEU:HD13	2.15	0.62
1:A:112:LYS:HE3	1:A:114:TYR:CZ	2.35	0.61
1:A:58:ARG:HH11	1:A:60:LEU:HD13	1.69	0.58
1:A:162:ASP:OD2	5:A:291:HOH:O	2.17	0.57
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.40	0.57
1:A:62:ASN:O	1:A:170:LYS:NZ	2.39	0.56
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.42	0.55
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.37	0.55
1:A:134:ALA:O	1:A:140:GLY:HA3	2.07	0.55
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.87	0.54
1:A:186:PRO:CG	1:A:212:LEU:HD23	2.38	0.53
1:A:252:LYS:O	1:A:253:ASN:CB	2.57	0.52
1:A:168:LYS:NZ	5:A:324:HOH:O	2.42	0.52
1:A:149:LYS:O	1:A:217:SER:HA	2.09	0.52
1:A:116:ALA:HB3	1:A:148:LEU:HD22	1.92	0.50
1:A:201:PRO:HA	1:A:203:LEU:HG	1.95	0.49
1:A:123:TRP:CZ3	1:A:125:THR:HA	2.49	0.48
1:A:125:THR:C	1:A:127:LYS:CA	2.83	0.48
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:O	1:A:82:GLY:HA2	2.13	0.48
1:A:164:LEU:HD22	1:A:229:LEU:HD21	1.97	0.47
1:A:150:VAL:HA	1:A:218:VAL:O	2.15	0.47
1:A:159:LYS:NZ	1:A:177:THR:O	2.47	0.47
1:A:137:GLN:HB3	1:A:138:PRO:HD2	1.97	0.46
1:A:58:ARG:CG	1:A:69:GLU:OE1	2.63	0.46
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.45	0.46
1:A:47:LEU:HD22	1:A:79:LEU:HD21	1.98	0.45
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.51	0.45
1:A:249:GLN:HB3	1:A:250:PRO:CD	2.46	0.45
1:A:41:ASP:O	1:A:44:LEU:HB2	2.16	0.45
1:A:45:LYS:HB3	1:A:46:PRO:HD2	1.99	0.45
1:A:167:ILE:HG13	1:A:167:ILE:O	2.17	0.45
1:A:253:ASN:C	1:A:253:ASN:ND2	2.66	0.44
1:A:219:SER:OG	1:A:222:GLN:HG3	2.16	0.44
1:A:193:THR:HA	1:A:209:TRP:O	2.19	0.43
1:A:112:LYS:HE3	1:A:114:TYR:CE2	2.53	0.43
1:A:88:TYR:OH	5:A:359:HOH:O	2.18	0.43
1:A:133:LYS:O	1:A:136:GLN:HB2	2.18	0.42
1:A:144:LEU:CD2	1:A:212:LEU:HD13	2.50	0.42
1:A:185:LEU:HA	1:A:186:PRO:HD3	1.97	0.42
1:A:29:SER:HB3	1:A:194:TYR:OH	2.20	0.42
1:A:124:ASN:OD1	1:A:127:LYS:N	2.54	0.41
1:A:160:VAL:O	1:A:163:VAL:HG12	2.20	0.41
1:A:186:PRO:HG2	1:A:212:LEU:HD23	2.03	0.41
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.80	0.41
1:A:112:LYS:CE	1:A:114:TYR:CZ	3.02	0.41
1:A:246:ARG:HA	1:A:247:PRO:HD3	1.84	0.41
1:A:8:GLY:O	1:A:12:GLY:N	2.54	0.40
1:A:161:VAL:HG13	1:A:225:LYS:HD3	2.04	0.40
1:A:249:GLN:HB3	1:A:250:PRO:HD2	2.03	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ASN:ND2	1:A:225:LYS:NZ[2_455]	1.56	0.64
1:A:58:ARG:NH1	1:A:238:GLU:O[2_555]	2.19	0.01

## 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	A	252/259 (97%)	234 (93%)	17 (7%)	1 (0%)	34	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN

### 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	A	221/224 (99%)	211 (96%)	10 (4%)	27	27

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	37	THR
1	A	39	LYS
1	A	44	LEU
1	A	58	ARG
1	A	79	LEU
1	A	92	GLN
1	A	100	LEU
1	A	144	LEU
1	A	253	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	67	ASN
1	A	137	GLN
1	A	253	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	AZM	A	264	2	8,13,13	1.04	1 (12%)	9,19,19	2.92	5 (55%)

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
4	AZM	A	264	2	-	0/2/10/10	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	264	AZM	S1-N1	-2.07	1.56	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	264	AZM	O2-S1-C1	-5.98	101.56	108.59
4	A	264	AZM	O2-S1-O1	3.51	124.53	118.76
4	A	264	AZM	O3-C3-C4	3.12	127.86	122.06
4	A	264	AZM	O3-C3-N4	-2.76	119.41	123.04
4	A	264	AZM	O2-S1-N1	2.07	110.43	107.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	264	AZM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	125:THR	C	127:LYS	N	2.20

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.