



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:16 AM EDT

PDB ID : 2CBE / pdb\_00002cbe  
Title : STRUCTURE OF NATIVE AND APO CARBONIC ANHYDRASE II AND SOME OF ITS ANION-LIGAND COMPLEXES  
Authors : Hakansson, K.; Carlsson, M.; Svensson, L.A.; Liljas, A.  
Deposited on : 1992-06-01  
Resolution : 1.82 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.

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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

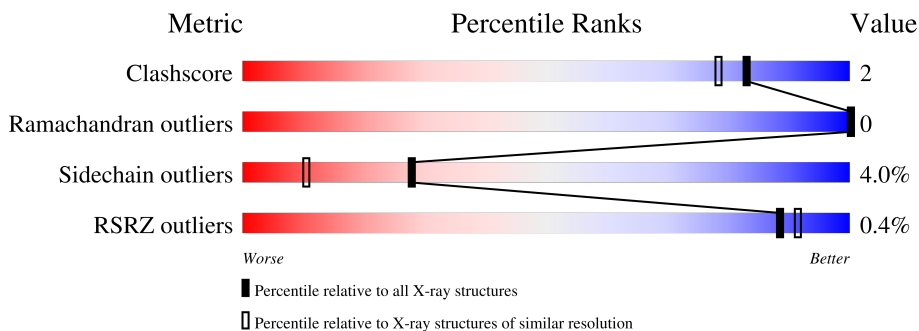
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.82 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	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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 of 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2297 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
			Total	C	N	O	S			
1	A	258	2079	1333	360	384	2	0	4	0

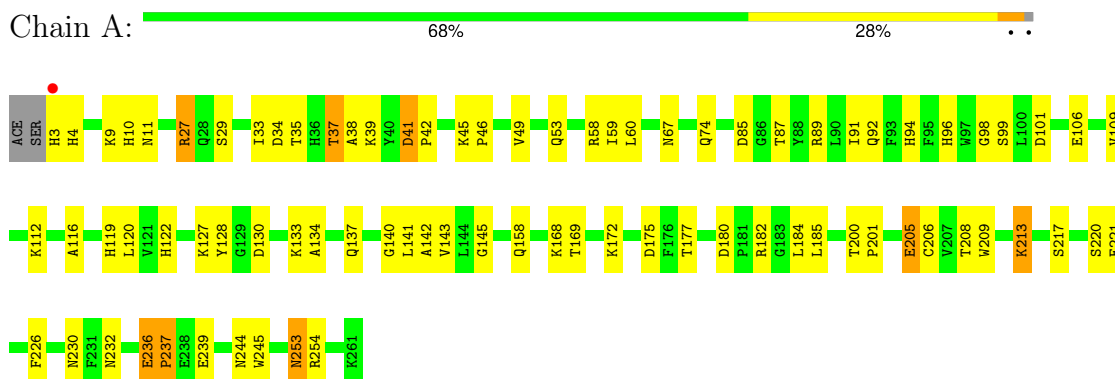
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	218	Total	O	0	0
			218	218		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: CARBONIC ANHYDRASE II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.70Å 41.70Å 73.00Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	10.00 – 1.82 10.00 – 1.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.82) 64.4 (10.00-1.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.83Å)	Xtrriage
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.158 , (Not available) 0.154 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.040 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2297	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<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.

## 5 Model quality i

### 5.1 Standard geometry i

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	1.52	10/2161 (0.5%)	2.05	75/2931 (2.6%)

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	2	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	THR	N-CA	9.36	1.53	1.45
1	A	245	TRP	N-CA	6.58	1.54	1.45
1	A	254	ARG	NE-CZ	6.40	1.40	1.33
1	A	120	LEU	C-O	6.04	1.31	1.24
1	A	34	ASP	N-CA	5.76	1.53	1.46
1	A	253	ASN	C-O	5.39	1.30	1.24
1	A	116	ALA	C-O	5.34	1.30	1.23
1	A	185	LEU	N-CA	5.23	1.53	1.46
1	A	205	GLU	CA-C	-5.12	1.47	1.53
1	A	87	THR	CA-CB	5.03	1.61	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ASN	CA-CB-CG	8.42	121.02	112.60
1	A	41	ASP	CB-CA-C	7.52	120.12	110.34
1	A	53	GLN	OE1-CD-NE2	7.52	130.12	122.60
1	A	158	GLN	OE1-CD-NE2	-7.33	115.28	122.60
1	A	58	ARG	N-CA-CB	-7.31	99.45	111.66
1	A	236	GLU	CB-CG-CD	7.23	124.89	112.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	HIS	CA-CB-CG	-7.17	106.63	113.80
1	A	98	GLY	O-C-N	7.04	130.90	123.09
1	A	180	ASP	CB-CA-C	6.83	117.75	110.17
1	A	67	ASN	CA-C-O	-6.79	112.98	120.38
1	A	3	HIS	CA-CB-CG	6.70	120.50	113.80
1	A	244	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	A	221	GLU	CG-CD-OE1	6.60	133.59	118.40
1	A	74	GLN	OE1-CD-NE2	6.60	129.20	122.60
1	A	53	GLN	CG-CD-NE2	-6.58	106.53	116.40
1	A	37	THR	CA-CB-CG2	6.55	121.64	110.50
1	A	168	LYS	CA-C-O	-6.47	113.69	120.55
1	A	226	PHE	CA-CB-CG	6.46	120.27	113.80
1	A	74	GLN	O-C-N	6.46	130.53	123.10
1	A	85	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	29	SER	CA-C-O	-6.26	114.22	120.66
1	A	236	GLU	CG-CD-OE1	6.24	132.75	118.40
1	A	142	ALA	CA-C-N	-6.21	115.00	123.14
1	A	142	ALA	C-N-CA	-6.21	115.00	123.14
1	A	119	HIS	CA-C-O	-6.19	113.51	120.32
1	A	87	THR	CA-CB-OG1	-6.14	100.38	109.60
1	A	133	LYS	O-C-N	6.04	130.08	122.23
1	A	130	ASP	OD1-CG-OD2	-6.03	108.43	122.90
1	A	237	PRO	CB-CA-C	5.94	119.13	111.46
1	A	106	GLU	CA-CB-CG	-5.90	102.30	114.10
1	A	91	ILE	CA-CB-CG2	5.88	120.50	110.50
1	A	27	ARG	CG-CD-NE	5.83	124.83	112.00
1	A	220	SER	CA-CB-OG	-5.83	99.43	111.10
1	A	99	SER	CA-C-N	5.82	131.64	122.21
1	A	99	SER	C-N-CA	5.82	131.64	122.21
1	A	253	ASN	N-CA-CB	-5.76	100.76	110.49
1	A	120	LEU	CA-C-O	-5.69	114.62	120.54
1	A	177	THR	CA-CB-OG1	-5.66	101.11	109.60
1	A	89	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	A	184	LEU	O-C-N	5.64	129.06	122.24
1	A	89	ARG	CB-CA-C	-5.60	100.30	109.53
1	A	27	ARG	CA-CB-CG	5.57	125.24	114.10
1	A	85	ASP	CA-C-N	-5.52	114.05	122.06
1	A	85	ASP	C-N-CA	-5.52	114.05	122.06
1	A	217	SER	CB-CA-C	-5.51	100.22	109.48
1	A	96	HIS	CA-C-O	-5.50	114.22	120.32
1	A	213	LYS	CG-CD-CE	5.45	123.84	111.30
1	A	4[A]	HIS	CA-CB-CG	-5.40	108.40	113.80

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4[B]	HIS	CA-CB-CG	-5.40	108.40	113.80
1	A	182	ARG	CA-CB-CG	-5.40	103.30	114.10
1	A	109	VAL	CA-C-O	-5.39	114.78	120.39
1	A	208	THR	N-CA-C	-5.38	99.01	108.20
1	A	217	SER	CA-CB-OG	-5.37	100.37	111.10
1	A	11	ASN	CA-C-N	5.36	128.22	121.36
1	A	11	ASN	C-N-CA	5.36	128.22	121.36
1	A	143	VAL	CA-C-O	-5.35	114.78	120.39
1	A	35	THR	O-C-N	5.33	128.82	122.27
1	A	59	ILE	CB-CA-C	5.33	118.71	110.50
1	A	175	ASP	N-CA-C	-5.33	102.51	110.23
1	A	53	GLN	CB-CG-CD	-5.29	103.61	112.60
1	A	141	LEU	N-CA-CB	-5.28	102.65	111.20
1	A	236	GLU	N-CA-CB	5.26	117.40	109.82
1	A	209	TRP	CE2-CD2-CE3	5.25	124.05	118.80
1	A	94	HIS	CA-C-O	-5.23	115.85	121.45
1	A	33	ILE	O-C-N	5.21	129.23	122.77
1	A	94	HIS	O-C-N	5.20	129.08	123.10
1	A	169	THR	CA-CB-OG1	-5.19	101.82	109.60
1	A	101	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	60	LEU	N-CA-CB	-5.13	101.95	111.13
1	A	94	HIS	CA-CB-CG	-5.12	108.68	113.80
1	A	122	HIS	CA-CB-CG	5.09	118.89	113.80
1	A	38	ALA	N-CA-C	-5.08	102.76	110.28
1	A	49	VAL	CA-C-O	-5.05	114.75	120.66
1	A	145	GLY	O-C-N	-5.05	118.23	123.48
1	A	232	ASN	CA-C-O	5.04	127.73	121.99

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4[A]	HIS	CA
1	A	4[B]	HIS	CA

There are no planarity outliers.

## 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	2079	0	2021	10	0
2	A	218	0	0	3	0
All	All	2297	0	2021	10	0

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 2.

All (10) 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:236:GLU:HB3	1:A:237:PRO:HD2	1.79	0.65
1:A:134:ALA:O	1:A:140:GLY:HA3	2.08	0.53
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.40	0.52
1:A:206:CYS:HB3	2:A:362:HOH:O	2.11	0.51
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.99	0.45
1:A:172:LYS:HE2	2:A:297:HOH:O	2.15	0.45
1:A:41:ASP:HA	1:A:42:PRO:HD2	1.89	0.43
1:A:112:LYS:NZ	2:A:423:HOH:O	2.52	0.42
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.55	0.41
1:A:45:LYS:HB3	1:A:46:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

## 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	260/260 (100%)	252 (97%)	8 (3%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 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	227/224 (101%)	218 (96%)	9 (4%)	28 10

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	37	THR
1	A	39	LYS
1	A	92	GLN
1	A	127	LYS
1	A	201	PRO
1	A	213	LYS
1	A	239	GLU
1	A	253	ASN

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

Mol	Chain	Res	Type
1	A	36	HIS
1	A	53	GLN
1	A	67	ASN
1	A	92	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 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<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	258/260 (99%)	-0.68	1 (0%) <b>88</b> <b>91</b>	4, 12, 26, 34	5 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.