



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 12:39 AM EST

PDB ID : 1CA2
Title : REFINED STRUCTURE OF HUMAN CARBONIC ANHYDRASE II AT 2.0
ANGSTROMS RESOLUTION
Authors : Eriksson, A.E.; Jones, T.A.; Liljas, A.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

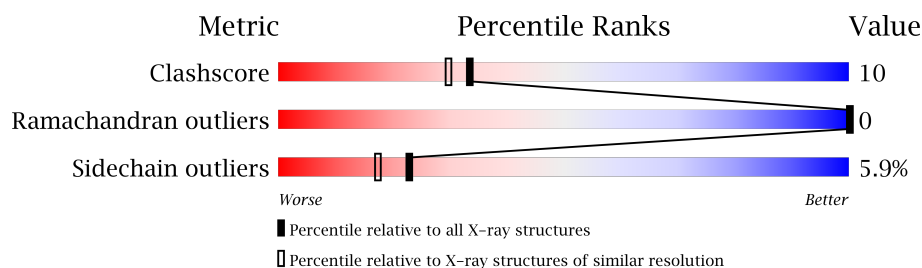
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2207 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
			2039	1309	350	378	2			

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	167	Total	O	0	0
			167	167		



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, α , β , γ	42.70 Å 41.70 Å 73.00 Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2207	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.39	7/2100 (0.3%)	1.78	46/2851 (1.6%)

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	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	18.11	1.75	1.34
1	A	63	GLY	C-N	7.08	1.50	1.34
1	A	227	ARG	CZ-NH1	5.93	1.40	1.33
1	A	260	PHE	C-O	5.44	1.33	1.23
1	A	58	ARG	CB-CG	-5.32	1.38	1.52
1	A	106	GLU	CD-OE1	-5.25	1.19	1.25
1	A	194	TYR	CG-CD2	5.03	1.45	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	NE-CZ-NH1	15.45	128.03	120.30
1	A	58	ARG	NE-CZ-NH2	-14.56	113.02	120.30
1	A	72	ASP	CB-CG-OD1	13.40	130.36	118.30
1	A	89	ARG	NE-CZ-NH2	-10.89	114.86	120.30
1	A	175	ASP	CB-CG-OD1	10.04	127.34	118.30
1	A	125	THR	C-N-CA	-9.11	98.91	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	A	58	ARG	CD-NE-CZ	7.83	134.57	123.60
1	A	221	GLU	CA-CB-CG	7.80	130.57	113.40
1	A	27	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	A	182	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	26	GLU	CG-CD-OE1	6.69	131.68	118.30
1	A	208	THR	N-CA-CB	6.35	122.36	110.30
1	A	58	ARG	CA-CB-CG	6.33	127.32	113.40
1	A	79	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	227	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	51	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	A	197	SER	N-CA-CB	-6.00	101.49	110.50
1	A	236	GLU	CG-CD-OE1	5.88	130.06	118.30
1	A	14	GLU	CB-CG-CD	5.88	130.07	114.20
1	A	19	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	101	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	190	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	27	ARG	CG-CD-NE	5.57	123.50	111.80
1	A	221	GLU	CG-CD-OE1	5.57	129.44	118.30
1	A	214	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	130	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	53	GLN	CA-CB-CG	-5.53	101.23	113.40
1	A	89	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	19	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	254	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	26	GLU	CG-CD-OE2	-5.41	107.49	118.30
1	A	72	ASP	OD1-CG-OD2	-5.38	113.08	123.30
1	A	27	ARG	CA-CB-CG	5.29	125.04	113.40
1	A	51	TYR	CB-CG-CD2	5.28	124.17	121.00
1	A	44	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	100	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	106	GLU	CG-CD-OE2	-5.24	107.81	118.30
1	A	166	SER	CB-CA-C	-5.20	100.21	110.10
1	A	165	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	133	LYS	CD-CE-NZ	-5.19	99.76	111.70
1	A	106	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	A	37	THR	CA-CB-CG2	5.15	119.61	112.40
1	A	221	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	A	175	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	221	GLU	N-CA-CB	5.02	119.64	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	PHE	Mainchain

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	2039	0	1988	39	1
2	A	1	0	0	0	0
3	A	167	0	0	5	1
All	All	2207	0	1988	39	1

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 10.

All (39) 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	1.75	1.36
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.57	1.03
1:A:125:THR:C	1:A:127:LYS:CA	2.44	0.86
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.22	0.74
1:A:75:ASP:OD1	1:A:89:ARG:NE	2.23	0.70
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.40	0.66
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.78	0.65
1:A:231:PHE:HD1	1:A:239:GLU:HG2	1.63	0.63
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.29	0.62
1:A:168:LYS:NZ	3:A:406:HOH:O	2.07	0.57
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.26	0.56
1:A:165:ASP:HB2	3:A:421:HOH:O	2.05	0.55
1:A:128:TYR:CE2	1:A:137:GLN:HG3	2.42	0.54
1:A:125:THR:O	1:A:127:LYS:CA	2.57	0.53
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.40	0.51
1:A:82:GLY:HA2	1:A:191:TYR:OH	2.11	0.51
1:A:231:PHE:CE2	1:A:241:MET:HG3	2.46	0.51
1:A:163:VAL:O	1:A:166:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:O	1:A:82:GLY:HA2	2.12	0.49
1:A:40:TYR:CE1	1:A:42:PRO:HB3	2.49	0.48
1:A:134:ALA:O	1:A:140:GLY:HA3	2.14	0.48
1:A:40:TYR:HE1	1:A:42:PRO:HB3	1.78	0.47
1:A:164:LEU:HB3	1:A:229:LEU:HD11	1.97	0.47
1:A:252:LYS:NZ	3:A:363:HOH:O	2.48	0.47
1:A:41:ASP:C	1:A:41:ASP:OD2	2.52	0.46
1:A:149:LYS:O	1:A:217:SER:HA	2.16	0.46
1:A:125:THR:O	1:A:127:LYS:HA	2.17	0.45
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.97	0.45
1:A:27:ARG:HD3	3:A:294:HOH:O	2.18	0.43
1:A:44:LEU:HD11	1:A:83:PRO:HB3	2.00	0.43
1:A:58:ARG:HG3	1:A:69:GLU:OE1	2.19	0.42
1:A:188:SER:HB3	1:A:214:GLU:OE2	2.20	0.42
1:A:220:SER:O	1:A:224:LEU:HG	2.20	0.42
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.81	0.42
1:A:128:TYR:CZ	1:A:137:GLN:HG3	2.55	0.42
1:A:206:CYS:HB3	3:A:362:HOH:O	2.18	0.41
1:A:59:ILE:HA	1:A:67:ASN:O	2.20	0.41
1:A:89:ARG:HG3	1:A:125:THR:HG22	2.02	0.41
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.22	0.40

All (1) 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:162:ASP:OD2	3:A:373:HOH:O[2_445]	1.97	0.23

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	254/259 (98%)	246 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	221/224 (99%)	208 (94%)	13 (6%)	23	17

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	39	LYS
1	A	53	GLN
1	A	58	ARG
1	A	60	LEU
1	A	79	LEU
1	A	80	LYS
1	A	83	PRO
1	A	127	LYS
1	A	202	PRO
1	A	221	GLU
1	A	229	LEU
1	A	255	GLN

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	136	GLN
1	A	137	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 carbohydrates in this entry.

5.6 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.

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	1.75

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.