



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:52 AM EDT

PDB ID : 1HUG / pdb_00001hug
Title : Differences in anionic inhibition of Human Carbonic Anhydrase I revealed from the structures of iodide and gold cyanide inhibitor complexes
Authors : Kumar, V.; Kannan, K.K.
Deposited on : 1993-10-28
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 ⓘ 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

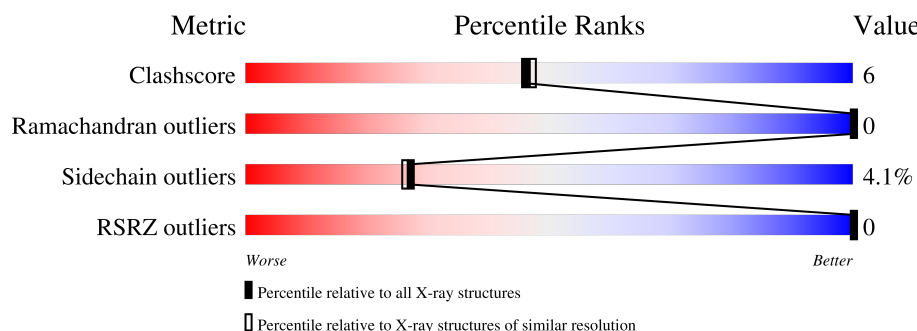
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2250 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.

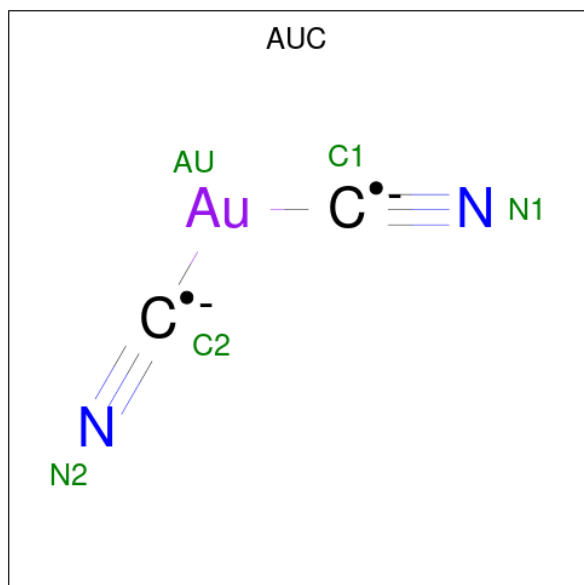
- Molecule 1 is a protein called CARBONIC ANHYDRASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2008	1270	349	386	3			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is GOLD (I) CYANIDE ION (CCD ID: AUC) (formula: C₂AuN₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Au	C	N	0	1
			5	1	2	2		
3	A	1	Total		Au			
			1		1			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Au		0	0
			1	1			
3	A	1	Total	Au	C	0	0
			3	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	231	Total	O	0	0
			231	231		

i

- Molecule 1: CARBONIC ANHYDRASE I

I216	E221	Q222	F226	R227	L230	S231	N232	V233	E234	M241	Q242	H243	R246	F260	K127	Y128	S129	S130	E133	A134	A135	A136	K137	G140	V143	I144	G145	V146	L147	M148	K149	L157	G158	K159	V160	L161	I167	T168	T169	K170	R173	A174	P175	F176	D180	P181	S188	L189	D190	T193	S197	L198	T199	H200	P201	S206	V207	T208	W209	L210	I211	ALA	SER	PRO	ASP	W5	D9	K10	M11	S17	K18	L19	I22	A23	N24	G25	N26	H27	Q28	V31	H40	K45	P46	I47	S48	A56	I59	I60	G63	E71	D72	N73	R76	K80	D86	Q92	F93	G98	N101	E102	A116	E117	W123
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.80Å 75.20Å 37.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 90.8 (8.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.171 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 102.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2250	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

5.1 Standard geometry

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

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	1.29	2/2065 (0.1%)	2.06	68/2808 (2.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ILE	C-N	-6.10	1.28	1.33
1	A	56	ALA	N-CA	5.14	1.52	1.46

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASP	CA-CB-CG	11.48	124.08	112.60
1	A	173	ARG	CD-NE-CZ	9.42	137.59	124.40
1	A	24	ASN	CA-CB-CG	9.32	121.92	112.60
1	A	200	HIS	O-C-N	8.49	129.44	121.71
1	A	226	PHE	O-C-N	7.96	130.27	122.07
1	A	233	VAL	CB-CA-C	7.88	122.51	111.63
1	A	86	ASP	CA-CB-CG	7.72	120.32	112.60
1	A	173	ARG	CG-CD-NE	7.43	128.34	112.00
1	A	86	ASP	CB-CA-C	7.36	124.08	110.24
1	A	71	GLU	CB-CG-CD	7.29	124.98	112.60
1	A	160	VAL	O-C-N	6.88	128.91	121.83
1	A	19	LEU	N-CA-C	6.75	122.19	113.88
1	A	221	GLU	CB-CG-CD	6.63	123.88	112.60
1	A	243	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	73	ASN	CA-CB-CG	6.37	118.97	112.60
1	A	198	LEU	N-CA-C	-6.37	101.52	110.50
1	A	209	TRP	O-C-N	6.37	130.52	123.01
1	A	221	GLU	N-CA-CB	6.28	120.02	110.28
1	A	130	SER	CA-C-O	-6.23	114.78	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ARG	CD-NE-CZ	6.19	133.07	124.40
1	A	140	GLY	N-CA-C	6.11	120.60	112.77
1	A	200	HIS	CA-C-O	-6.09	114.47	120.26
1	A	146	VAL	O-C-N	6.06	129.80	123.26
1	A	176	PHE	CA-C-O	-5.95	112.89	120.27
1	A	31	VAL	O-C-N	5.95	129.74	123.02
1	A	136	SER	CA-C-O	-5.89	112.31	119.32
1	A	102	GLU	CA-C-N	-5.86	114.28	123.13
1	A	102	GLU	C-N-CA	-5.86	114.28	123.13
1	A	175	PRO	N-CA-C	-5.82	101.95	111.21
1	A	60	ILE	CA-C-O	5.80	127.14	120.76
1	A	246	ARG	NH1-CZ-NH2	-5.74	111.83	119.30
1	A	180	ASP	CA-C-O	5.73	124.86	119.59
1	A	157	LEU	CA-C-N	5.69	128.22	120.54
1	A	157	LEU	C-N-CA	5.69	128.22	120.54
1	A	130	SER	N-CA-CB	-5.66	102.74	111.46
1	A	127	LYS	N-CA-C	5.64	120.29	112.90
1	A	26	ASN	O-C-N	5.61	129.35	122.34
1	A	173	ARG	NH1-CZ-NH2	5.54	126.51	119.30
1	A	160	VAL	N-CA-CB	5.46	118.78	110.58
1	A	181	PRO	CB-CA-C	5.46	119.68	111.44
1	A	246	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	28	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	A	40	HIS	O-C-N	5.41	129.77	122.96
1	A	136	SER	O-C-N	5.37	128.74	122.24
1	A	190	ASP	CA-CB-CG	-5.33	107.27	112.60
1	A	174	ALA	O-C-N	5.32	127.48	122.06
1	A	116	ALA	O-C-N	5.31	128.67	122.99
1	A	207	VAL	O-C-N	5.28	128.52	123.14
1	A	207	VAL	N-CA-C	5.27	116.18	108.53
1	A	11	ASN	O-C-N	5.24	129.28	122.15
1	A	222	GLN	OE1-CD-NE2	5.21	127.81	122.60
1	A	123	TRP	CB-CA-C	5.20	119.58	109.33
1	A	197	SER	N-CA-C	5.18	116.17	108.86
1	A	147	LEU	CB-CA-C	5.18	118.29	109.53
1	A	133	GLU	CA-C-N	5.16	127.19	120.28
1	A	133	GLU	C-N-CA	5.16	127.19	120.28
1	A	47	ILE	CB-CA-C	5.15	118.66	111.34
1	A	143	VAL	CA-C-N	-5.15	115.73	122.37
1	A	143	VAL	C-N-CA	-5.15	115.73	122.37
1	A	211	ILE	N-CA-CB	5.13	117.21	111.21
1	A	241	MET	CA-C-N	5.11	127.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	MET	C-N-CA	5.11	127.13	120.28
1	A	159	LYS	CA-C-N	5.10	127.67	120.42
1	A	159	LYS	C-N-CA	5.10	127.67	120.42
1	A	161	LEU	O-C-N	5.08	127.50	122.12
1	A	117	GLU	CA-C-O	5.07	127.06	120.21
1	A	227	ARG	CB-CG-CD	5.02	122.84	111.30
1	A	234	GLU	CA-C-O	-5.01	115.63	121.15

There are no chirality outliers.

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	2008	0	1935	23	0
2	A	1	0	0	0	0
3	A	10	0	0	1	0
4	A	231	0	0	2	0
All	All	2250	0	1935	23	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 6.

All (23) 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:26:ASN:HD22	3:A:503:AUC:C2	1.93	0.81
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.69	0.74
1:A:101:ASN:OD1	1:A:227:ARG:NH2	2.22	0.65
1:A:127:LYS:HD3	4:A:311:HOH:O	2.03	0.57
1:A:17:SER:O	1:A:18:LYS:C	2.50	0.55
1:A:149:LYS:HG3	4:A:444:HOH:O	2.07	0.54
1:A:45:LYS:HB3	1:A:46:PRO:HD2	1.91	0.53
1:A:47:ILE:HD11	1:A:189:LEU:HD13	1.90	0.53
1:A:200:HIS:HB2	1:A:201:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HD12	1:A:173:ARG:HB3	1.93	0.50
1:A:128:TYR:CE1	1:A:137:LYS:HG3	2.46	0.50
1:A:193:THR:HA	1:A:209:TRP:O	2.14	0.48
1:A:134:ALA:O	1:A:140:GLY:HA3	2.15	0.47
1:A:92:GLN:HG2	1:A:93:PHE:N	2.30	0.46
1:A:167:ILE:HG13	1:A:167:ILE:O	2.15	0.45
1:A:230:LEU:HB3	1:A:232:ASN:OD1	2.17	0.45
1:A:80:LYS:HE3	1:A:80:LYS:HB2	1.82	0.43
1:A:148:MET:HA	1:A:216:ILE:O	2.19	0.43
1:A:17:SER:C	1:A:19:LEU:N	2.76	0.42
1:A:63:GLY:HA3	1:A:170:LYS:HD2	2.02	0.42
1:A:137:LYS:O	1:A:206:SER:HB2	2.21	0.41
1:A:169:THR:HG21	1:A:234:GLU:HA	2.02	0.41
1:A:98:GLY:HA2	1:A:243:HIS:HB2	2.01	0.41

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	254/260 (98%)	242 (95%)	12 (5%)	0	100	100

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	222/225 (99%)	213 (96%)	9 (4%)	27	26

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

Mol	Chain	Res	Type
1	A	19	LEU
1	A	22	ILE
1	A	48	SER
1	A	60	ILE
1	A	76	ARG
1	A	188	SER
1	A	221	GLU
1	A	227	ARG
1	A	233	VAL

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	11	ASN
1	A	15	GLN
1	A	26	ASN
1	A	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic and 2 are modelled with single atom - 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 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	$\# Z > 2$
3	AUC	A	500[A]	-	4,4,4	2.63	2 (50%)	-		
3	AUC	A	503	-	2,2,4	0.91	0	-		

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500[A]	AUC	AU-C2	3.97	2.27	1.97
3	A	500[A]	AUC	C2-N2	2.50	1.29	1.14

There are no bond angle outliers.

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
3	A	503	AUC	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	256/260 (98%)	-0.80	0 100 100	5, 16, 33, 53	0

There are no RSRZ outliers to report.

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](#)

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, 95th 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	B-factors(Å ²)	Q<0.9
3	AUC	A	503	3/5	0.90	0.10	54,54,55,58	1
3	AUC	A	502	1/5	0.91	0.05	38,38,38,38	1
3	AUC	A	501[B]	1/5	0.98	0.05	12,12,12,12	1
3	AUC	A	500[A]	5/5	0.99	0.07	17,18,20,22	3
2	ZN	A	261	1/1	1.00	0.06	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.