



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:00 PM UTC

PDB ID : 1HEB / pdb_00001heb
Title : STRUCTURAL CONSEQUENCES OF HYDROPHILIC AMINO-ACID
SUBSTITUTIONS IN THE HYDROPHOBIC POCKET OF HUMAN CAR-
BONIC ANHYDRASE II
Authors : Nair, S.K.; Christianson, D.W.
Deposited on : 1992-07-16
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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

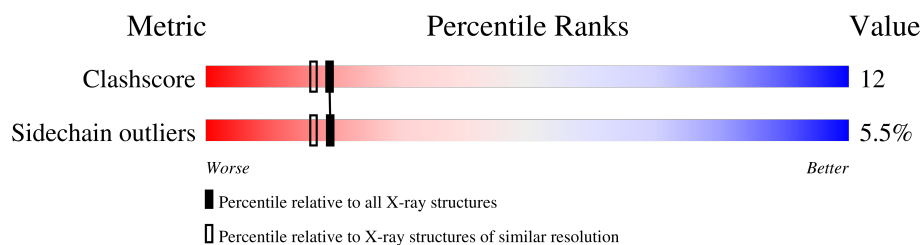
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	260	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2139 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	255	Total	C	N	O	S	0	0	0
			2030	1302	347	379	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	GLU	LEU	conflict	UNP P00918

- 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 MERCURY (II) ION (CCD ID: HG) (formula: Hg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total	O	0	0
			107	107		

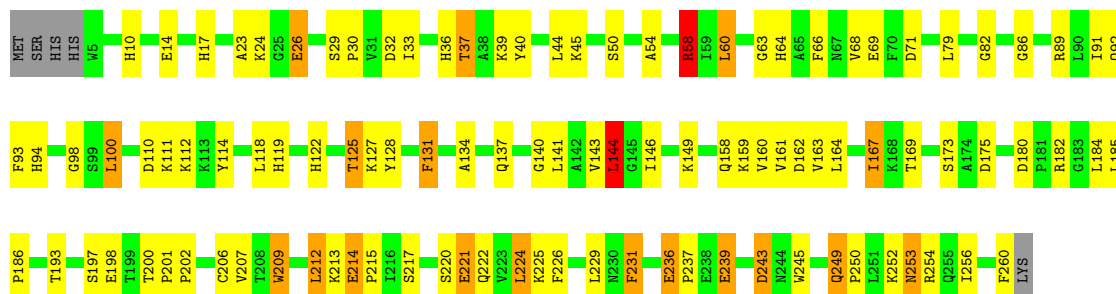
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: CARBONIC ANHYDRASE II

Chain A: 



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}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2139	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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, 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	2.13	26/2090 (1.2%)	2.13	66/2837 (2.3%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	48.45	1.98	1.33
1	A	119	HIS	CE1-NE2	7.70	1.40	1.32
1	A	206	CYS	CA-CB	7.38	1.64	1.53
1	A	94	HIS	CE1-NE2	7.16	1.39	1.32
1	A	10	HIS	CE1-NE2	6.75	1.39	1.32
1	A	64	HIS	ND1-CE1	-6.51	1.26	1.32
1	A	144	LEU	C-N	-6.47	1.27	1.33
1	A	222	GLN	C-O	6.33	1.31	1.24
1	A	66	PHE	C-N	-6.32	1.25	1.33
1	A	184	LEU	C-O	6.17	1.32	1.23
1	A	201	PRO	CA-C	-6.00	1.46	1.52
1	A	98	GLY	N-CA	6.00	1.50	1.44
1	A	36	HIS	C-N	-5.94	1.25	1.33
1	A	256	ILE	N-CA	5.86	1.53	1.46
1	A	26	GLU	CD-OE2	5.84	1.36	1.25
1	A	173	SER	C-O	5.84	1.31	1.23
1	A	64	HIS	CE1-NE2	5.70	1.38	1.32
1	A	164	LEU	C-O	5.67	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CD-OE2	5.54	1.35	1.25
1	A	175	ASP	C-O	5.52	1.30	1.23
1	A	17	HIS	C-N	-5.43	1.26	1.33
1	A	54	ALA	C-N	5.31	1.40	1.33
1	A	36	HIS	C-O	5.28	1.30	1.24
1	A	33	ILE	CA-CB	-5.27	1.47	1.53
1	A	50	SER	CA-C	5.25	1.60	1.53
1	A	118	LEU	C-O	5.12	1.30	1.24

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	SER	O-C-N	17.14	136.54	121.80
1	A	29	SER	CA-C-O	-15.80	102.61	120.46
1	A	201	PRO	CA-C-O	-12.32	102.69	120.56
1	A	201	PRO	O-C-N	10.93	134.35	121.46
1	A	202	PRO	N-CD-CG	9.79	115.55	103.80
1	A	125	THR	CA-C-N	-9.57	103.19	120.99
1	A	125	THR	C-N-CA	-9.57	103.19	120.99
1	A	26	GLU	CB-CG-CD	9.25	128.33	112.60
1	A	10	HIS	CA-CB-CG	-8.53	105.27	113.80
1	A	207	VAL	N-CA-C	8.35	120.30	108.36
1	A	30	PRO	CA-N-CD	-8.18	100.05	111.50
1	A	201	PRO	CB-CA-C	7.96	120.63	110.92
1	A	226	PHE	CA-CB-CG	7.94	121.74	113.80
1	A	14	GLU	CB-CG-CD	7.87	125.98	112.60
1	A	30	PRO	N-CD-CG	7.59	112.90	103.80
1	A	32	ASP	O-C-N	7.46	131.72	123.22
1	A	202	PRO	N-CA-CB	7.43	110.77	102.60
1	A	214	GLU	CA-C-O	7.35	124.76	119.32
1	A	231	PHE	CA-CB-CG	7.32	121.12	113.80
1	A	30	PRO	N-CA-CB	7.25	110.57	102.60
1	A	24	LYS	O-C-N	6.72	131.05	121.97
1	A	92	GLN	O-C-N	6.55	129.84	123.29
1	A	200	THR	O-C-N	6.44	126.45	121.88
1	A	224	LEU	CA-C-N	6.38	129.46	120.28
1	A	224	LEU	C-N-CA	6.38	129.46	120.28
1	A	202	PRO	CA-N-CD	-6.31	102.66	111.50
1	A	93	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	63	GLY	CA-C-O	-6.28	112.38	119.04
1	A	212	LEU	O-C-N	6.10	130.33	122.89
1	A	100	LEU	CA-CB-CG	6.08	137.58	116.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	CA-C-O	-6.06	114.48	121.15
1	A	249	GLN	O-C-N	6.03	126.63	121.20
1	A	198	GLU	N-CA-C	-5.97	102.65	110.53
1	A	141	LEU	N-CA-C	5.87	119.12	109.85
1	A	209	TRP	O-C-N	5.83	129.86	123.22
1	A	231	PHE	N-CA-C	-5.71	105.14	111.36
1	A	243	ASP	CA-CB-CG	-5.71	106.89	112.60
1	A	197	SER	N-CA-C	5.65	117.56	109.14
1	A	159	LYS	O-C-N	5.64	128.10	122.12
1	A	158	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	A	119	HIS	O-C-N	5.54	129.70	123.27
1	A	207	VAL	CB-CA-C	-5.53	103.31	110.84
1	A	63	GLY	O-C-N	5.50	129.38	122.28
1	A	236	GLU	O-C-N	5.49	126.01	121.35
1	A	131	PHE	CA-C-N	5.42	126.92	120.14
1	A	131	PHE	C-N-CA	5.42	126.92	120.14
1	A	239	GLU	CA-CB-CG	5.42	124.94	114.10
1	A	37	THR	CA-CB-OG1	-5.39	101.52	109.60
1	A	91	ILE	CB-CA-C	5.33	116.13	110.91
1	A	66	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	26	GLU	CG-CD-OE1	5.26	130.50	118.40
1	A	68	VAL	N-CA-CB	5.25	118.08	111.46
1	A	93	PHE	N-CA-C	-5.25	101.32	109.24
1	A	167	ILE	CA-C-N	5.20	127.20	120.44
1	A	167	ILE	C-N-CA	5.20	127.20	120.44
1	A	23	ALA	CA-C-N	-5.17	115.47	123.17
1	A	23	ALA	C-N-CA	-5.17	115.47	123.17
1	A	40	TYR	CA-C-O	-5.13	114.80	120.70
1	A	169	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	24	LYS	CA-CB-CG	5.12	124.34	114.10
1	A	10	HIS	ND1-CG-CD2	5.12	111.22	106.10
1	A	186	PRO	CB-CA-C	5.11	118.94	111.22
1	A	162	ASP	CA-C-O	-5.06	114.38	120.10
1	A	185	LEU	CA-C-O	5.06	124.44	120.19
1	A	122	HIS	CA-CB-CG	5.04	118.84	113.80
1	A	143	VAL	O-C-N	5.04	128.54	123.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2030	0	1975	47	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	107	0	0	1	1
All	All	2139	0	1975	47	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 12.

All (47) 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	1.98	1.22
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.64	0.97
1:A:253:ASN:C	1:A:253:ASN:HD22	1.77	0.93
1:A:144:LEU:HD22	1:A:212:LEU:HD21	1.61	0.83
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.15	0.76
1:A:253:ASN:HD22	1:A:254:ARG:N	1.86	0.73
1:A:144:LEU:HD22	1:A:212:LEU:CD2	2.21	0.71
1:A:253:ASN:ND2	1:A:254:ARG:N	2.39	0.70
1:A:250:PRO:HB2	1:A:252:LYS:HG3	1.77	0.67
1:A:253:ASN:C	1:A:253:ASN:ND2	2.45	0.66
1:A:160:VAL:O	1:A:163:VAL:HG12	1.95	0.66
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.76	0.66
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.22	0.65
1:A:134:ALA:O	1:A:140:GLY:HA3	2.00	0.62
1:A:125:THR:C	1:A:127:LYS:CA	2.72	0.61
1:A:144:LEU:CD2	1:A:212:LEU:HD21	2.30	0.61
1:A:252:LYS:O	1:A:253:ASN:CG	2.44	0.60
1:A:112:LYS:HE3	1:A:114:TYR:CE1	2.40	0.56
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.71	0.56
1:A:60:LEU:HD21	1:A:69:GLU:OE2	2.06	0.55
1:A:131:PHE:O	1:A:134:ALA:HB3	2.09	0.53
1:A:146:ILE:HG12	1:A:212:LEU:HD23	1.92	0.52
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:CD2	1:A:69:GLU:OE2	2.58	0.51
1:A:249:GLN:HB3	1:A:250:PRO:HD2	1.94	0.48
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.50	0.48
1:A:221:GLU:H	1:A:221:GLU:CD	2.22	0.47
1:A:45:LYS:O	1:A:82:GLY:HA2	2.15	0.47
1:A:89:ARG:HG3	1:A:125:THR:HG22	1.98	0.46
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.50	0.46
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.46	0.46
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.51	0.46
1:A:146:ILE:CG1	1:A:212:LEU:HD23	2.44	0.46
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.98	0.45
1:A:252:LYS:O	1:A:253:ASN:CB	2.65	0.44
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.53	0.43
1:A:220:SER:O	1:A:224:LEU:HG	2.18	0.43
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.78	0.42
1:A:221:GLU:O	1:A:225:LYS:HG3	2.19	0.42
1:A:193:THR:HA	1:A:209:TRP:O	2.20	0.42
1:A:149:LYS:O	1:A:217:SER:HA	2.20	0.41
1:A:110:ASP:O	1:A:111:LYS:HB2	2.20	0.41
1:A:167:ILE:O	1:A:167:ILE:HG13	2.21	0.41
1:A:71:ASP:OD1	1:A:71:ASP:C	2.63	0.41
1:A:86:GLY:HA3	4:A:290:HOH:O	2.22	0.40
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.99	0.40
1:A:180:ASP:CG	1:A:182:ARG:HE	2.30	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)
4:A:294:HOH:O	4:A:321:HOH:O[2_445]	1.96	0.24

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	220/225 (98%)	208 (94%)	12 (6%)	19	17

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	37	THR
1	A	39	LYS
1	A	44	LEU
1	A	58	ARG
1	A	60	LEU
1	A	79	LEU
1	A	100	LEU
1	A	144	LEU
1	A	221	GLU
1	A	229	LEU
1	A	253	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	67	ASN
1	A	137	GLN
1	A	178	ASN
1	A	253	ASN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are 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	1.98

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.