



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:18 PM UTC

PDB ID : 1HED / pdb_00001hed
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

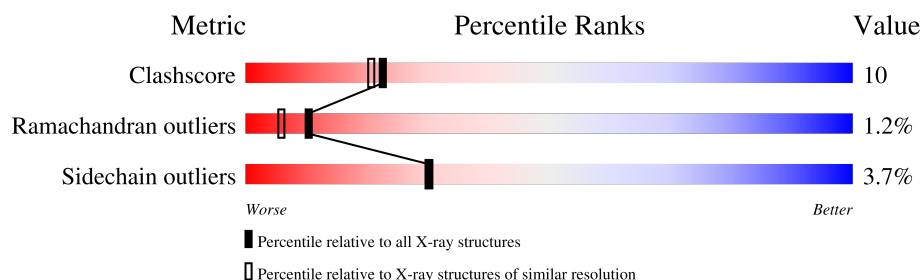
1 Overall quality at a glance

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)
Ramachandran outliers	187476	11031 (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 2136 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
			2026	1300	347	377	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ALA	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	2	Total	Hg	0	0
			2	2		

- Molecule 4 is water.

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

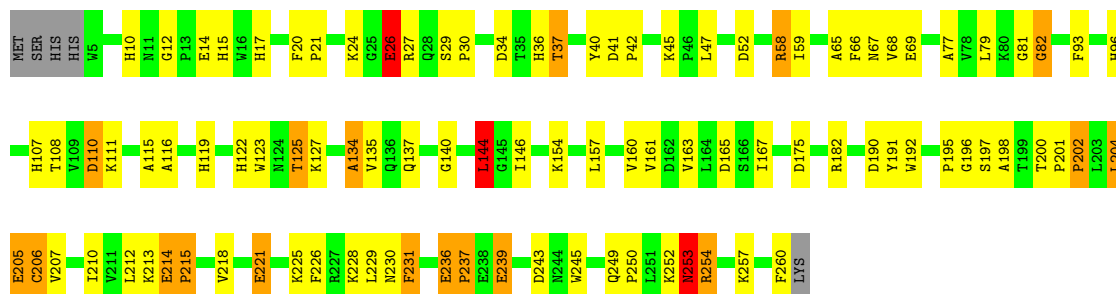
3 Residue-property plots

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}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2136	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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	2.18	34/2086 (1.6%)	2.10	63/2832 (2.2%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	49.22	1.99	1.33
1	A	196	GLY	N-CA	9.44	1.53	1.45
1	A	201	PRO	C-O	-7.76	1.15	1.24
1	A	214	GLU	CA-C	-7.39	1.44	1.52
1	A	236	GLU	CA-CB	-6.61	1.44	1.53
1	A	36	HIS	CE1-NE2	6.58	1.39	1.32
1	A	119	HIS	CE1-NE2	6.41	1.39	1.32
1	A	108	THR	CA-C	6.38	1.60	1.52
1	A	110	ASP	CA-C	6.05	1.60	1.53
1	A	65	ALA	C-O	5.89	1.29	1.24
1	A	20	PHE	N-CA	5.87	1.53	1.46
1	A	116	ALA	C-O	5.85	1.30	1.23
1	A	239	GLU	CD-OE2	5.85	1.36	1.25
1	A	192	TRP	C-O	5.80	1.30	1.23
1	A	253	ASN	C-O	5.78	1.31	1.24
1	A	257	LYS	C-O	5.71	1.30	1.23
1	A	205	GLU	CA-C	-5.70	1.47	1.53
1	A	34	ASP	N-CA	5.62	1.53	1.46
1	A	17	HIS	CE1-NE2	5.51	1.38	1.32
1	A	204	LEU	C-N	-5.48	1.26	1.33
1	A	154	LYS	CA-CB	-5.47	1.45	1.53
1	A	115	ALA	C-O	5.39	1.30	1.24
1	A	82	GLY	N-CA	5.39	1.52	1.44
1	A	182	ARG	N-CA	5.39	1.53	1.46
1	A	215	PRO	N-CD	5.33	1.55	1.47
1	A	26	GLU	N-CA	-5.26	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ALA	N-CA	5.26	1.52	1.46
1	A	68	VAL	CA-C	5.25	1.59	1.52
1	A	52	ASP	C-O	5.20	1.30	1.24
1	A	144	LEU	C-O	5.20	1.30	1.24
1	A	66	PHE	C-O	5.18	1.30	1.24
1	A	230	ASN	N-CA	5.11	1.52	1.45
1	A	205	GLU	CD-OE2	5.07	1.34	1.25
1	A	10	HIS	CG-CD2	5.04	1.41	1.35

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	SER	O-C-N	16.56	136.04	121.80
1	A	29	SER	CA-C-O	-15.57	102.87	120.46
1	A	201	PRO	O-C-N	14.27	138.30	121.46
1	A	201	PRO	CA-C-O	-14.18	100.00	120.56
1	A	202	PRO	N-CD-CG	10.06	115.87	103.80
1	A	30	PRO	CA-N-CD	-9.39	98.35	111.50
1	A	30	PRO	N-CD-CG	9.39	115.07	103.80
1	A	30	PRO	N-CA-CB	8.96	112.46	102.60
1	A	214	GLU	CA-C-N	8.88	129.01	120.31
1	A	214	GLU	C-N-CA	8.88	129.01	120.31
1	A	125	THR	CA-C-N	-8.72	104.77	120.99
1	A	125	THR	C-N-CA	-8.72	104.77	120.99
1	A	202	PRO	CA-N-CD	-8.49	99.61	111.50
1	A	207	VAL	N-CA-C	8.22	120.95	108.71
1	A	226	PHE	CA-CB-CG	8.12	121.92	113.80
1	A	125	THR	CA-C-O	8.00	129.16	120.20
1	A	202	PRO	N-CA-CB	7.93	111.33	102.60
1	A	239	GLU	CA-CB-CG	7.92	129.95	114.10
1	A	14	GLU	CB-CG-CD	7.79	125.85	112.60
1	A	231	PHE	CA-CB-CG	7.63	121.43	113.80
1	A	201	PRO	CB-CA-C	7.28	119.80	110.92
1	A	231	PHE	N-CA-C	-7.13	102.54	112.45
1	A	122	HIS	ND1-CE1-NE2	6.48	114.88	108.40
1	A	198	ALA	CA-C-O	-6.44	114.54	121.56
1	A	230	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	15	HIS	ND1-CE1-NE2	6.26	114.66	108.40
1	A	110	ASP	N-CA-C	-6.22	103.08	111.54
1	A	41	ASP	CA-C-N	6.07	126.18	119.87
1	A	41	ASP	C-N-CA	6.07	126.18	119.87
1	A	249	GLN	O-C-N	5.98	126.43	121.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	THR	CA-CB-OG1	-5.97	100.64	109.60
1	A	236	GLU	CA-CB-CG	5.92	125.94	114.10
1	A	125	THR	O-C-N	-5.88	115.50	122.20
1	A	122	HIS	ND1-CG-CD2	5.74	111.84	106.10
1	A	93	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	26	GLU	N-CA-C	5.69	119.40	112.23
1	A	81	GLY	O-C-N	5.67	128.29	122.90
1	A	24	LYS	O-C-N	5.62	129.56	121.97
1	A	12	GLY	CA-C-N	5.60	125.71	119.32
1	A	12	GLY	C-N-CA	5.60	125.71	119.32
1	A	175	ASP	CA-C-O	-5.49	115.15	121.19
1	A	200	THR	O-C-N	5.47	125.77	121.88
1	A	107	HIS	ND1-CE1-NE2	5.42	113.82	108.40
1	A	230	ASN	CB-CG-ND2	5.40	124.50	116.40
1	A	165	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	66	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	119	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
1	A	191	TYR	CA-C-O	5.32	127.14	121.45
1	A	195	PRO	O-C-N	5.32	129.83	122.64
1	A	77	ALA	O-C-N	5.30	130.12	123.12
1	A	197	SER	N-CA-C	5.27	116.99	109.14
1	A	82	GLY	CA-C-N	5.24	126.26	120.45
1	A	82	GLY	C-N-CA	5.24	126.26	120.45
1	A	157	LEU	CA-C-N	5.21	127.27	120.28
1	A	157	LEU	C-N-CA	5.21	127.27	120.28
1	A	237	PRO	CB-CA-C	5.20	118.25	111.64
1	A	154	LYS	CA-C-N	5.18	124.63	119.24
1	A	154	LYS	C-N-CA	5.18	124.63	119.24
1	A	206	CYS	O-C-N	5.14	128.26	122.20
1	A	96	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	119	HIS	CA-C-O	-5.06	114.88	120.30
1	A	218	VAL	CB-CA-C	5.06	118.24	110.55
1	A	228	LYS	CA-C-O	5.06	125.27	119.35

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	2026	0	1974	42	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	107	0	0	2	0
All	All	2136	0	1974	42	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 10.

All (42) 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	1.99	1.19
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.57	1.03
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.11	0.86
1:A:253:ASN:HD22	1:A:254:ARG:N	1.85	0.75
1:A:253:ASN:HD22	1:A:253:ASN:C	1.96	0.73
1:A:253:ASN:ND2	1:A:254:ARG:N	2.41	0.69
1:A:26:GLU:OE1	1:A:205:GLU:OE1	2.09	0.69
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.40	0.65
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.77	0.65
1:A:252:LYS:O	1:A:253:ASN:CG	2.42	0.62
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.25	0.61
1:A:144:LEU:HD22	1:A:212:LEU:HD21	1.82	0.61
1:A:45:LYS:O	1:A:82:GLY:HA2	2.00	0.60
1:A:146:ILE:HG12	1:A:212:LEU:HD23	1.82	0.60
1:A:253:ASN:C	1:A:253:ASN:ND2	2.60	0.59
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.67	0.59
1:A:125:THR:C	1:A:127:LYS:CA	2.76	0.58
1:A:110:ASP:O	1:A:111:LYS:HB2	2.06	0.54
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.38	0.54
1:A:213:LYS:HD3	1:A:260:PHE:CE1	2.42	0.52
1:A:144:LEU:HD22	1:A:212:LEU:CD2	2.41	0.50
1:A:134:ALA:O	1:A:140:GLY:HA3	2.12	0.50
1:A:26:GLU:CD	1:A:26:GLU:H	2.19	0.49
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.95	0.48
1:A:190:ASP:HB3	1:A:260:PHE:CD2	2.49	0.48
1:A:59:ILE:HA	1:A:67:ASN:O	2.13	0.48
1:A:146:ILE:CG1	1:A:212:LEU:HD23	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.96	0.46
1:A:202:PRO:HG2	1:A:204:LEU:HG	1.99	0.45
1:A:239:GLU:HB2	4:A:370:HOH:O	2.17	0.44
1:A:160:VAL:O	1:A:163:VAL:HG12	2.18	0.44
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.75	0.43
1:A:253:ASN:O	1:A:254:ARG:C	2.62	0.43
1:A:123:TRP:CZ3	1:A:125:THR:HA	2.54	0.43
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.53	0.43
1:A:137:GLN:O	1:A:206:CYS:HB3	2.19	0.42
1:A:250:PRO:HB2	1:A:252:LYS:HG3	2.01	0.42
1:A:221:GLU:H	1:A:221:GLU:CD	2.28	0.41
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.50	0.41
1:A:40:TYR:CE2	1:A:42:PRO:HG3	2.55	0.41
1:A:21:PRO:HD2	4:A:272:HOH:O	2.22	0.40
1:A:47:LEU:HD11	1:A:210:ILE:HG21	2.02	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	253/260 (97%)	240 (95%)	10 (4%)	3 (1%)	10 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	254	ARG
1	A	135	VAL

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	219/224 (98%)	211 (96%)	8 (4%)	30	30

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	37	THR
1	A	58	ARG
1	A	79	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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	137	GLN
1	A	178	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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	1.99

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.