



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:34 pm BST

PDB ID : 1HEB
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 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	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

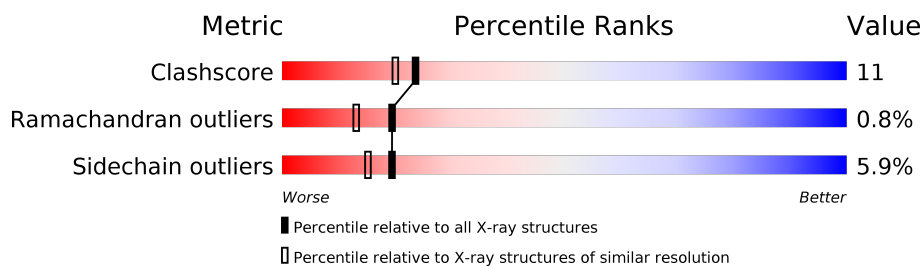
1 Overall quality at a glance

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

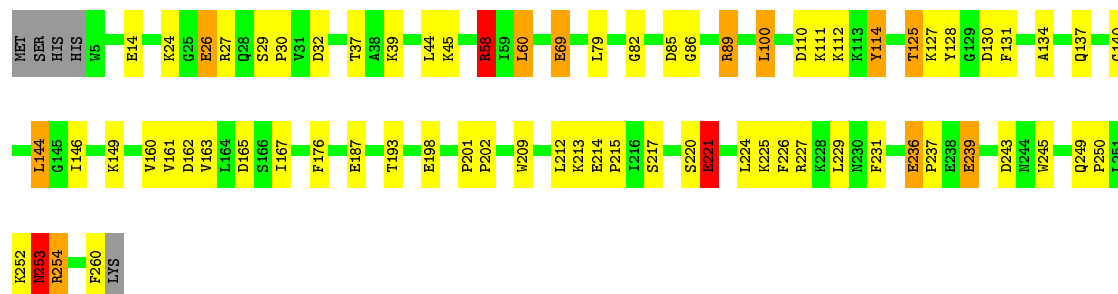
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Hg	0	0
			1	1		

- Molecule 4 is water.

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

Note EDS was not executed.

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	1.61	9/2090 (0.4%)	1.70	33/2837 (1.2%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	27.95	1.98	1.34
1	A	26	GLU	CD-OE2	9.82	1.36	1.25
1	A	236	GLU	CD-OE2	9.29	1.35	1.25
1	A	198	GLU	CD-OE2	7.72	1.34	1.25
1	A	14	GLU	CD-OE1	7.44	1.33	1.25
1	A	221	GLU	CD-OE2	-7.35	1.17	1.25
1	A	26	GLU	CD-OE1	-7.06	1.17	1.25
1	A	187	GLU	CD-OE1	6.42	1.32	1.25
1	A	69	GLU	CD-OE1	-5.71	1.19	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	NE-CZ-NH1	11.27	125.93	120.30
1	A	89	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	A	100	LEU	CA-CB-CG	9.69	137.58	115.30
1	A	58	ARG	NE-CZ-NH1	9.12	124.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASP	CB-CG-OD1	8.66	126.09	118.30
1	A	227	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	29	SER	CA-C-O	-8.33	102.61	120.10
1	A	202	PRO	N-CD-CG	8.23	115.55	103.20
1	A	30	PRO	CA-N-CD	-8.18	100.05	111.50
1	A	29	SER	O-C-N	8.12	136.54	121.10
1	A	130	ASP	CB-CG-OD1	7.92	125.43	118.30
1	A	125	THR	C-N-CA	-7.40	103.19	121.70
1	A	201	PRO	CA-C-O	-7.30	102.69	120.20
1	A	162	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	201	PRO	O-C-N	6.97	134.35	121.10
1	A	30	PRO	N-CD-CG	6.47	112.90	103.20
1	A	202	PRO	CA-N-CD	-6.31	102.66	111.50
1	A	202	PRO	N-CA-CB	6.23	110.77	103.30
1	A	26	GLU	CG-CD-OE1	6.10	130.50	118.30
1	A	30	PRO	N-CA-CB	6.06	110.57	103.30
1	A	114	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	A	32	ASP	O-C-N	5.64	131.72	122.70
1	A	58	ARG	CD-NE-CZ	5.54	131.35	123.60
1	A	27	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	239	GLU	CA-CB-CG	5.25	124.94	113.40
1	A	165	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	26	GLU	CB-CG-CD	5.23	128.33	114.20
1	A	226	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	A	69	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	A	226	PHE	CB-CG-CD1	5.13	124.39	120.80
1	A	85	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	176	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	A	26	GLU	OE1-CD-OE2	-5.06	117.23	123.30

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	45	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	45	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 11.

All (45) 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	1.17
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.64	0.97
1:A:253:ASN:HD22	1:A:253:ASN:C	1.77	0.88
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:253:ASN:C	1:A:253:ASN:ND2	2.45	0.69
1:A:250:PRO:HB2	1:A:252:LYS:HG3	1.77	0.67
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:134:ALA:O	1:A:140:GLY:HA3	2.00	0.62
1:A:144:LEU:CD2	1:A:212:LEU:HD21	2.30	0.61
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.22	0.60
1:A:125:THR:C	1:A:127:LYS:CA	2.72	0.57
1:A:112:LYS:HE3	1:A:114:TYR:CE1	2.40	0.56
1:A:252:LYS:O	1:A:253:ASN:CG	2.44	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:221:GLU:CD	1:A:221:GLU:H	2.22	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:HG13	1:A:167:ILE:O	2.21	0.41
1:A:144:LEU:HA	1:A:144:LEU:HD23	1.99	0.40
1:A:86:GLY:HA3	4:A:290:HOH:O	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)
4:A:294:HOH:O	4:A:321:HOH:O[2_445]	1.96	0.24

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%)	237 (94%)	14 (6%)	2 (1%)	19	13

All (2) Ramachandran outliers are listed below:

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

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	220/225 (98%)	207 (94%)	13 (6%)	19	15

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

Mol	Chain	Res	Type
1	A	24	LYS
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

Some 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	136	GLN
1	A	137	GLN
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 carbohydrates 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.