Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 06:02 PM EST

PDB ID	:	1CVA
Title	:	STRUCTURAL AND FUNCTIONAL IMPORTANCE OF A CONSERVED HYDROGEN BOND NETWORK IN HUMAN CARBONIC ANHYDRASE II
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Deposited on	:	1993-02-04
Resolution	:	2.25 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 (i) 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 (i)) were used in the production of this report:

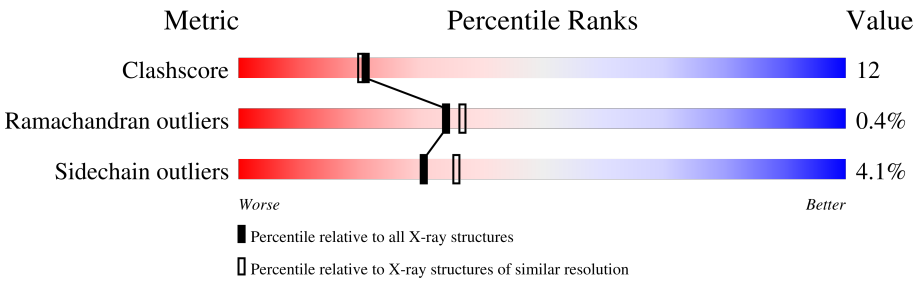
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	63% 30% 5% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AZI	A	357	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2127 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
			Total	C	N	O	S			
1	A	255	2029	1304	347	376	2	0	0	0

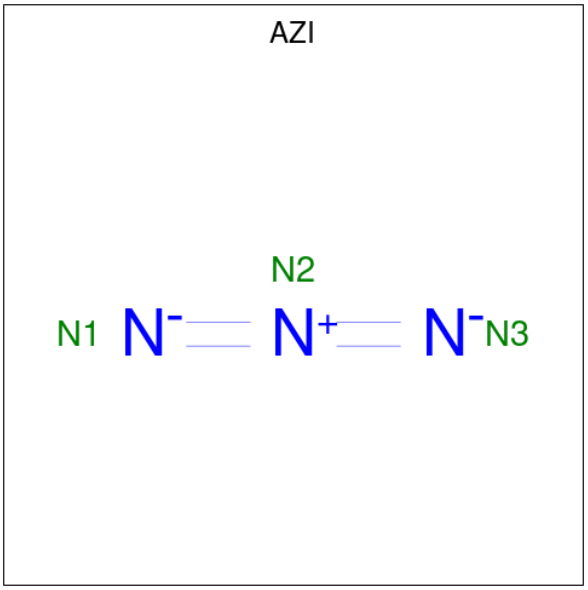
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	VAL	THR	conflict	UNP P00918

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N_3).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	94	94	94	0	0

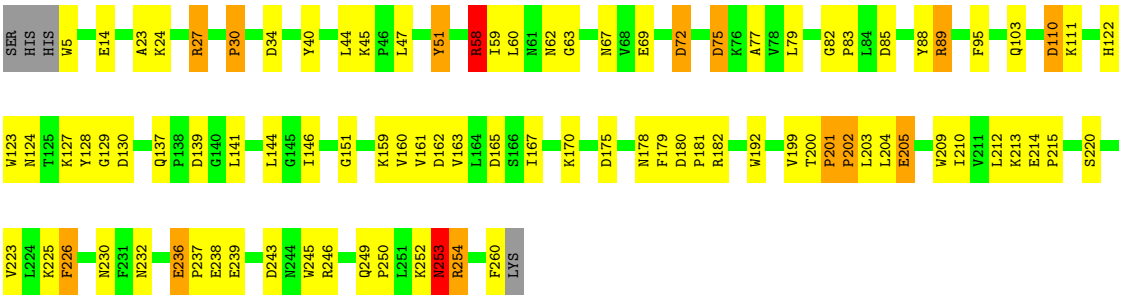
3 Residue-property plots (i)

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: 63% 30% 5% • •



4 Data and refinement statistics (i)

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	42.70Å 41.70Å 73.00Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	6.50 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (6.50-2.25)	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	2127	wwPDB-VP
Average B, all atoms ($Å^2$)	14.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.51	14/2089 (0.7%)	1.65	27/2836 (1.0%)

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	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	GLU	CD-OE1	8.64	1.35	1.25
1	A	238	GLU	CD-OE1	8.41	1.34	1.25
1	A	236	GLU	CD-OE2	7.31	1.33	1.25
1	A	129	GLY	N-CA	-6.75	1.35	1.46
1	A	236	GLU	CD-OE1	-6.64	1.18	1.25
1	A	205	GLU	CD-OE2	6.00	1.32	1.25
1	A	238	GLU	CD-OE2	-5.90	1.19	1.25
1	A	192	TRP	CD2-CE2	5.53	1.48	1.41
1	A	95	PHE	CE2-CZ	5.39	1.47	1.37
1	A	226	PHE	CG-CD2	5.34	1.46	1.38
1	A	14	GLU	CD-OE2	-5.33	1.19	1.25
1	A	151	GLY	CA-C	5.31	1.60	1.51
1	A	215	PRO	N-CD	5.19	1.55	1.47
1	A	214	GLU	CD-OE2	-5.10	1.20	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	ARG	NE-CZ-NH1	10.65	125.63	120.30
1	A	89	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	A	85	ASP	CB-CG-OD2	8.42	125.88	118.30
1	A	27	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	202	PRO	CA-N-CD	-7.82	100.55	111.50
1	A	51	TYR	CB-CG-CD1	7.82	125.69	121.00
1	A	72	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	202	PRO	N-CA-CB	7.06	111.77	103.30
1	A	75	ASP	CB-CG-OD1	6.84	124.45	118.30
1	A	58	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	201	PRO	CA-C-O	-6.16	105.41	120.20
1	A	30	PRO	CA-N-CD	-6.10	102.96	111.50
1	A	209	TRP	CD1-CG-CD2	6.07	111.15	106.30
1	A	202	PRO	N-CD-CG	6.03	112.24	103.20
1	A	89	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	110	ASP	CB-CG-OD2	5.93	123.63	118.30
1	A	40	TYR	CB-CG-CD1	-5.86	117.49	121.00
1	A	239	GLU	CA-CB-CG	5.64	125.80	113.40
1	A	175	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	34	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	139	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	175	ASP	CB-CA-C	5.22	120.84	110.40
1	A	130	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	236	GLU	CG-CD-OE2	-5.11	108.09	118.30
1	A	182	ARG	CD-NE-CZ	-5.07	116.50	123.60
1	A	141	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	23	ALA	O-C-N	5.05	130.77	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ARG	Sidechain
1	A	58	ARG	Sidechain

5.2 Too-close contacts (i)

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	2029	0	1984	49	1
2	A	1	0	0	0	0
3	A	3	0	0	2	0
4	A	94	0	0	3	1
All	All	2127	0	1984	49	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 (49) 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:58:ARG:HD2	1:A:69:GLU:OE1	1.46	1.15
1:A:63:GLY:HA3	1:A:170:LYS:HZ3	1.33	0.91
1:A:253:ASN:HD22	1:A:254:ARG:N	1.77	0.82
1:A:165:ASP:HB2	4:A:304:HOH:O	1.86	0.75
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.17	0.74
1:A:253:ASN:ND2	1:A:254:ARG:N	2.35	0.73
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.03	0.72
1:A:253:ASN:HD22	1:A:253:ASN:C	1.94	0.70
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.75	0.67
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.31	0.66
1:A:250:PRO:HB2	1:A:252:LYS:HG3	1.82	0.61
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.84	0.60
1:A:62:ASN:O	1:A:170:LYS:NZ	2.33	0.60
1:A:110:ASP:O	1:A:111:LYS:HB2	2.02	0.59
1:A:128:TYR:CZ	1:A:137:GLN:HG3	2.38	0.59
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.40	0.56
1:A:253:ASN:ND2	1:A:253:ASN:C	2.59	0.56
1:A:249:GLN:HB3	1:A:250:PRO:CD	2.36	0.56
1:A:160:VAL:O	1:A:163:VAL:HG12	2.06	0.56
1:A:45:LYS:O	1:A:82:GLY:HA2	2.08	0.54
1:A:202:PRO:HG2	1:A:204:LEU:HG	1.90	0.54
1:A:159:LYS:HE2	1:A:179:PHE:HD1	1.72	0.53
1:A:103:GLN:NE2	1:A:243:ASP:OD1	2.44	0.51
1:A:201:PRO:HA	1:A:203:LEU:HG	1.93	0.51
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.46	0.50
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.94	0.50
1:A:47:LEU:HD11	1:A:210:ILE:HG21	1.94	0.49
1:A:249:GLN:HB3	1:A:250:PRO:HD2	1.94	0.49
1:A:75:ASP:OD1	1:A:89:ARG:NE	2.41	0.47
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.45	0.46
1:A:199:VAL:HG22	3:A:357:AZI:N3	2.31	0.46
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.50	0.45
1:A:199:VAL:HG22	3:A:357:AZI:N2	2.31	0.45
1:A:72:ASP:OD2	1:A:123:TRP:NE1	2.42	0.45
1:A:159:LYS:HD2	4:A:308:HOH:O	2.17	0.45
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.18	0.44
1:A:59:ILE:HA	1:A:67:ASN:O	2.18	0.44
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.39	0.43
1:A:88:TYR:CE2	1:A:124:ASN:HB2	2.53	0.43
1:A:223:VAL:O	1:A:226:PHE:HB2	2.19	0.43
1:A:89:ARG:O	1:A:122:HIS:HA	2.20	0.42
1:A:60:LEU:HD21	1:A:67:ASN:HB2	2.02	0.42
1:A:51:TYR:CD1	1:A:77:ALA:HB1	2.55	0.42
1:A:167:ILE:O	1:A:167:ILE:HG13	2.19	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.87	0.41
1:A:178:ASN:HB2	4:A:325:HOH:O	2.22	0.40
1:A:146:ILE:HG12	1:A:212:LEU:HD12	2.04	0.40
1:A:5:TRP:CH2	1:A:200:THR:HB	2.55	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	4:A:352:HOH:O[2_445]	2.00	0.20

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	253/259 (98%)	237 (94%)	15 (6%)	1 (0%)	34 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN

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	220/224 (98%)	211 (96%)	9 (4%)	30 36

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

Mol	Chain	Res	Type
1	A	24	LYS
1	A	30	PRO
1	A	44	LEU
1	A	58	ARG
1	A	79	LEU
1	A	83	PRO
1	A	127	LYS
1	A	220	SER
1	A	253	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	AZI	A	357	2	0,2,2	-	-	0,1,1	-	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	357	AZI	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.