Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 02:00 PM EST

PDB ID	:	1CAL
Title	:	STRUCTURAL ANALYSIS OF THE ZINC HYDROXIDE-THR 199-GLU 106 HYDROGEN BONDING NETWORK IN HUMAN CARBONIC ANHYDRASE II
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Deposited on	:	1992-09-17
Resolution	:	2.20 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 (1)) were used in the production of this report:

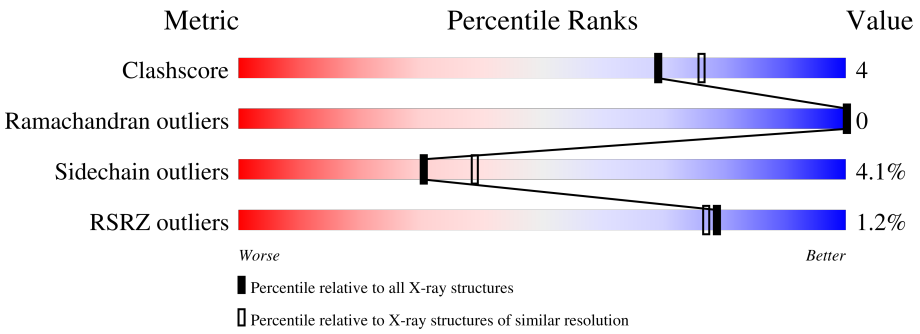
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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

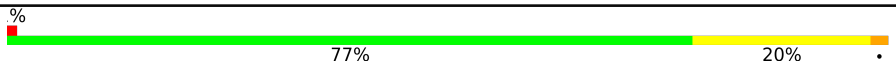
The reported resolution of this entry is 2.20 Å.

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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 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	259	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2281 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	258	2071	1328	358	383	2	0	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	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 water.

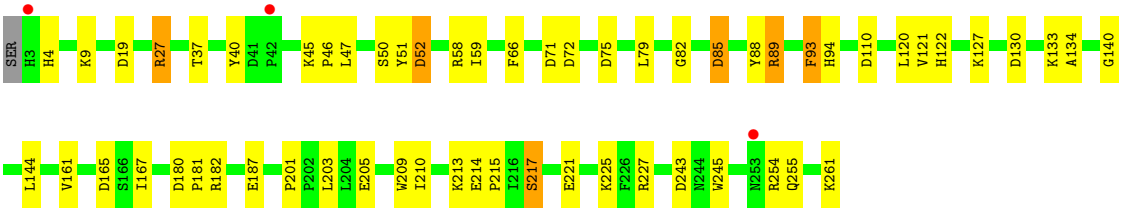
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	209	209	209	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

- Molecule 1: CARBONIC ANHYDRASE II

Chain A:



4 Data and refinement statistics (i)

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)	(Not available) – 2.20 24.02 – 2.08	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20) 63.5 (24.02-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.08Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.166 , (Not available) 0.150 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 84.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2281	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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

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	1.09	1/2148 (0.0%)	1.77	41/2913 (1.4%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	TRP	CD2-CE2	-5.21	1.35	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	ARG	NE-CZ-NH1	13.75	127.18	120.30
1	A	89	ARG	NE-CZ-NH2	-12.74	113.93	120.30
1	A	130	ASP	CB-CG-OD1	11.89	129.00	118.30
1	A	89	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	A	182	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	A	27	ARG	CG-CD-NE	10.32	133.48	111.80
1	A	75	ASP	CB-CG-OD1	9.45	126.80	118.30
1	A	254	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	165	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	A	88	TYR	CB-CG-CD1	8.01	125.81	121.00
1	A	52	ASP	CB-CG-OD1	7.47	125.02	118.30
1	A	19	ASP	CB-CG-OD1	7.47	125.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	TYR	CB-CG-CD2	-7.43	116.54	121.00
1	A	85	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	144	LEU	CA-CB-CG	6.97	131.32	115.30
1	A	221	GLU	CG-CD-OE1	6.82	131.95	118.30
1	A	37	THR	CA-CB-CG2	6.77	121.88	112.40
1	A	51	TYR	CB-CG-CD1	6.69	125.01	121.00
1	A	19	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	58	ARG	N-CA-CB	-6.59	98.75	110.60
1	A	209	TRP	CH2-CZ2-CE2	-6.55	110.85	117.40
1	A	4[A]	HIS	CA-CB-CG	6.24	124.22	113.60
1	A	4[B]	HIS	CA-CB-CG	6.24	124.22	113.60
1	A	71	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	A	217	SER	N-CA-CB	6.04	119.56	110.50
1	A	227	ARG	CD-NE-CZ	5.93	131.90	123.60
1	A	187	GLU	OE1-CD-OE2	5.90	130.38	123.30
1	A	133	LYS	O-C-N	5.87	132.09	122.70
1	A	93	PHE	N-CA-CB	5.71	120.88	110.60
1	A	72	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	4[A]	HIS	C-N-CA	5.51	135.49	121.70
1	A	4[B]	HIS	C-N-CA	5.51	135.49	121.70
1	A	51	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	A	85	ASP	N-CA-CB	5.46	120.42	110.60
1	A	133	LYS	N-CA-CB	5.45	120.41	110.60
1	A	110	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	227	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	187	GLU	CG-CD-OE1	-5.20	107.90	118.30
1	A	94	HIS	CA-CB-CG	-5.17	104.81	113.60
1	A	221	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	A	121	VAL	O-C-N	5.06	130.80	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	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	2071	0	2016	15	0
2	A	1	0	0	0	0
3	A	209	0	0	0	0
All	All	2281	0	2016	15	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 4.

All (15) 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:47:LEU:HD22	1:A:79:LEU:HD11	1.76	0.67
1:A:45:LYS:HB3	1:A:46:PRO:HD2	1.85	0.59
1:A:201:PRO:HA	1:A:203:LEU:HG	1.94	0.49
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.48	0.49
1:A:40:TYR:CE2	1:A:261:LYS:HE3	2.48	0.48
1:A:45:LYS:O	1:A:82:GLY:HA2	2.14	0.48
1:A:134:ALA:O	1:A:140:GLY:HA3	2.15	0.47
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.98	0.45
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.98	0.45
1:A:59:ILE:HD11	1:A:66:PHE:CD1	2.52	0.44
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.93	0.44
1:A:161:VAL:HG13	1:A:225:LYS:HD2	2.01	0.43
1:A:47:LEU:HD11	1:A:210:ILE:HG21	2.01	0.42
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.82	0.42
1:A:93:PHE:HB3	1:A:120:LEU:HD23	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	259/259 (100%)	249 (96%)	10 (4%)	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	225/223 (101%)	216 (96%)	9 (4%)	31	40

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

Mol	Chain	Res	Type
1	A	9	LYS
1	A	50	SER
1	A	52	ASP
1	A	85	ASP
1	A	122	HIS
1	A	127	LYS
1	A	213	LYS
1	A	217	SER
1	A	255	GLN

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	3	HIS
1	A	17	HIS
1	A	67	ASN
1	A	137	GLN

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 1 ligands modelled in this entry, 1 is 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)

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	258/259 (99%)	-0.84	3 (1%) 79 77	5, 17, 31, 39	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ASN	2.6
1	A	42	PRO	2.5
1	A	3	HIS	2.2

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 monosaccharides 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
2	ZN	A	262	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.