Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:48 AM GMT

PDB ID	:	3CA2
Title	:	CRYSTALLOGRAPHIC STUDIES OF INHIBITOR BINDING SITES IN HUMAN CARBONIC ANHYDRASE II. A PENTACOORDINATED BINDING OF THE SCN-ION TO THE ZINC AT HIGH P*H
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Deposited on	:	1989-10-02
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

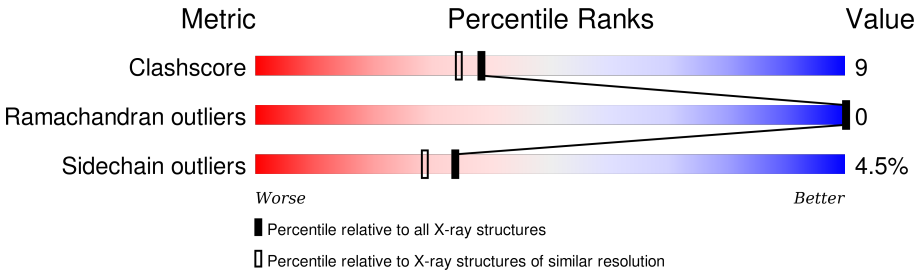
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	64% 30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2214 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	256	Total	C	N	O	S	0	0	0
			2039	1309	350	378	2			

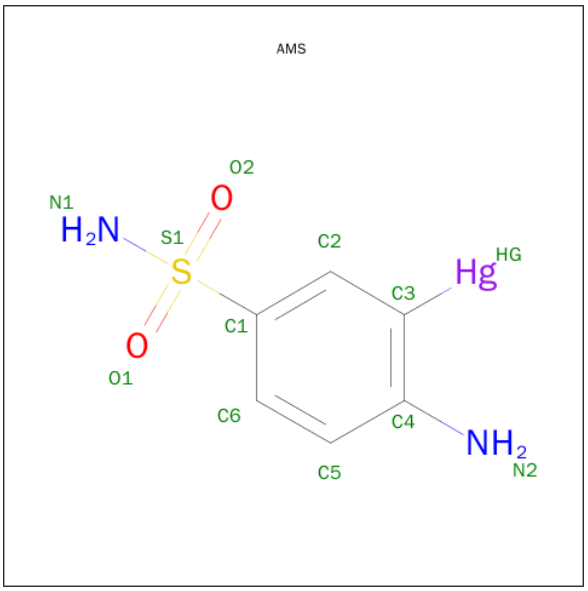
- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Hg	0	0
			2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is 3-MERCURI-4-AMINOBENZENESULFONAMIDE (three-letter code: AMS) (formula: $C_6H_7HgN_2O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Hg	N	O	S	0	0
			12	6	1	2	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total	O	0	0
			160	160		

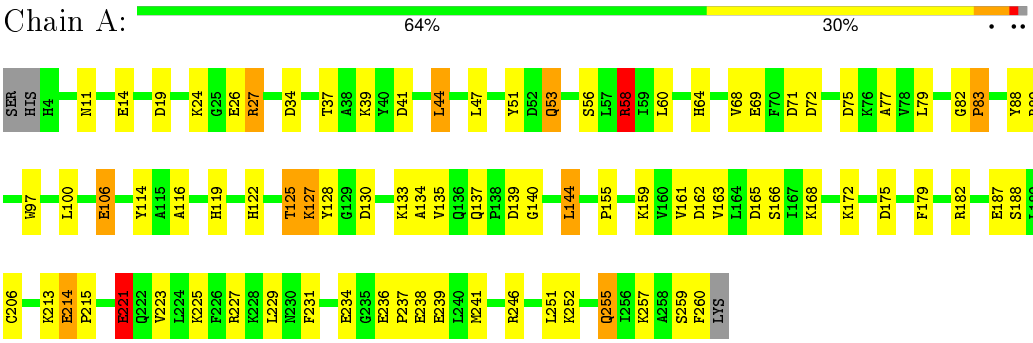
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: CARBONIC ANHYDRASE II

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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)	(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}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2214	wwPDB-VP
Average B, all atoms (Å^2)	9.0	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, AMS

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	1.56	10/2100 (0.5%)	1.92	57/2851 (2.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	21.61	1.83	1.34
1	A	246	ARG	CD-NE	6.72	1.57	1.46
1	A	259	SER	CB-OG	6.19	1.50	1.42
1	A	97	TRP	NE1-CE2	5.83	1.45	1.37
1	A	56	SER	CB-OG	5.64	1.49	1.42
1	A	58	ARG	CD-NE	-5.53	1.37	1.46
1	A	14	GLU	CD-OE1	5.41	1.31	1.25
1	A	187	GLU	CD-OE1	5.39	1.31	1.25
1	A	188	SER	CB-OG	-5.15	1.35	1.42
1	A	234	GLU	CD-OE1	-5.15	1.20	1.25

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	ASP	CB-CG-OD1	14.66	131.49	118.30
1	A	58	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	A	58	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	A	89	ARG	NE-CZ-NH2	-10.59	115.01	120.30
1	A	89	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	182	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	A	51	TYR	CB-CG-CD1	-9.47	115.32	121.00
1	A	125	THR	C-N-CA	-8.98	99.26	121.70
1	A	58	ARG	CD-NE-CZ	8.68	135.75	123.60
1	A	34	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	100	LEU	CA-CB-CG	7.52	132.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	11	ASN	C-N-CA	7.39	137.81	122.30
1	A	72	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	51	TYR	CB-CG-CD2	7.30	125.38	121.00
1	A	214	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	A	27	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	130	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	223	VAL	CG1-CB-CG2	-7.00	99.71	110.90
1	A	175	ASP	CB-CG-OD2	-6.88	112.10	118.30
1	A	44	LEU	CA-CB-CG	6.76	130.84	115.30
1	A	26	GLU	CG-CD-OE1	6.55	131.40	118.30
1	A	172	LYS	CA-CB-CG	6.50	127.70	113.40
1	A	238	GLU	CG-CD-OE1	6.50	131.29	118.30
1	A	41	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	26	GLU	CG-CD-OE2	-6.41	105.47	118.30
1	A	227	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	A	71	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	89	ARG	CD-NE-CZ	-6.22	114.89	123.60
1	A	77	ALA	CB-CA-C	6.20	119.40	110.10
1	A	75	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	A	106	GLU	CG-CD-OE2	-6.16	105.97	118.30
1	A	246	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	221	GLU	CA-CB-CG	6.04	126.68	113.40
1	A	116	ALA	O-C-N	6.01	132.32	122.70
1	A	27	ARG	CA-CB-CG	5.87	126.31	113.40
1	A	58	ARG	CG-CD-NE	5.86	124.11	111.80
1	A	190	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	165	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	144	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	182	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	179	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	A	155	PRO	O-C-N	5.61	132.74	123.20
1	A	89	ARG	CB-CA-C	-5.55	99.29	110.40
1	A	71	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	114	TYR	CB-CG-CD1	5.51	124.31	121.00
1	A	47	LEU	O-C-N	5.46	131.43	122.70
1	A	133	LYS	CA-CB-CG	5.38	125.24	113.40
1	A	106	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	A	127	LYS	CA-C-O	-5.38	108.81	120.10
1	A	19	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	162	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	93	PHE	CB-CG-CD2	-5.15	117.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	PHE	N-CA-CB	5.09	119.77	110.60
1	A	68	VAL	N-CA-C	-5.07	97.33	111.00
1	A	251	LEU	CB-CA-C	5.05	119.80	110.20
1	A	64	HIS	CG-ND1-CE1	5.03	115.24	108.20

There are no chirality outliers.

There are no planarity outliers.

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	2039	0	1987	35	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	12	0	8	2	0
5	A	160	0	0	6	0
All	All	2214	0	1995	37	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 9.

All (37) 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	1.83	1.31
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.42	1.18
4:A:265:AMS:C3	4:A:265:AMS:HG	1.78	0.91
4:A:265:AMS:HG	4:A:265:AMS:HG	0.84	0.83
1:A:125:THR:C	1:A:127:LYS:CA	2.50	0.80
1:A:252:LYS:NZ	5:A:362:HOH:O	2.22	0.73
1:A:135:VAL:O	1:A:206:CYS:SG	2.49	0.71
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.31	0.70
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.23	0.68
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.30	0.67
1:A:159:LYS:HE3	5:A:423:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:NZ	5:A:403:HOH:O	2.23	0.63
1:A:159:LYS:CE	5:A:423:HOH:O	2.47	0.63
1:A:255:GLN:OE1	1:A:257:LYS:HE2	2.05	0.57
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.23	0.56
1:A:44:LEU:HD11	1:A:83:PRO:HB3	1.88	0.56
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.36	0.55
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.87	0.54
1:A:137:GLN:O	1:A:206:CYS:HB3	2.09	0.51
1:A:231:PHE:HD1	1:A:239:GLU:HG2	1.76	0.50
1:A:231:PHE:CE2	1:A:241:MET:HG3	2.47	0.49
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.95	0.49
1:A:128:TYR:CE2	1:A:137:GLN:HG3	2.48	0.48
1:A:24:LYS:NZ	5:A:425:HOH:O	2.49	0.46
1:A:134:ALA:O	1:A:140:GLY:HA3	2.17	0.45
1:A:163:VAL:O	1:A:166:SER:HB2	2.17	0.45
1:A:37:THR:HG22	5:A:375:HOH:O	2.17	0.45
1:A:139:ASP:OD2	1:A:139:ASP:N	2.49	0.44
1:A:53:GLN:HB2	1:A:53:GLN:HE21	1.42	0.44
1:A:88:TYR:HB3	1:A:122:HIS:HB3	2.00	0.44
1:A:236:GLU:HB3	1:A:237:PRO:HD2	2.00	0.42
1:A:82:GLY:HA2	1:A:191:TYR:OH	2.20	0.41
1:A:44:LEU:HG	1:A:191:TYR:OH	2.20	0.41
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.81	0.41
1:A:221:GLU:O	1:A:225:LYS:HG3	2.21	0.41
1:A:106:GLU:OE1	1:A:119:HIS:HE1	2.03	0.41
1:A:91:ILE:HG23	1:A:92:GLN:HG3	2.04	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	254/259 (98%)	244 (96%)	10 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	221/224 (99%)	211 (96%)	10 (4%)	34 29

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	53	GLN
1	A	58	ARG
1	A	60	LEU
1	A	79	LEU
1	A	83	PRO
1	A	144	LEU
1	A	221	GLU
1	A	229	LEU
1	A	255	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

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

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are 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	$\#\|Z\| > 2$
4	AMS	A	265	1,3,5	9,12,12	2.50	5 (55%)	14,18,18	6.31	6 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMS	A	265	1,3,5	-	0/6/6/6	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	265	AMS	C5-C4	2.25	1.46	1.40
4	A	265	AMS	C1-S1	2.47	1.80	1.77
4	A	265	AMS	C6-C1	3.26	1.44	1.38
4	A	265	AMS	C6-C5	3.71	1.45	1.38
4	A	265	AMS	C2-C1	4.35	1.47	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	265	AMS	O2-S1-O1	-14.06	99.04	118.80
4	A	265	AMS	O1-S1-N1	-7.61	97.42	107.28
4	A	265	AMS	O2-S1-N1	-7.02	98.19	107.28
4	A	265	AMS	O2-S1-C1	8.83	118.27	107.39
4	A	265	AMS	O1-S1-C1	9.13	118.64	107.39
4	A	265	AMS	C1-S1-N1	9.25	120.70	108.45

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
4	A	265	AMS	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.