



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2016 – 12:07 PM EDT

PDB ID : 5JJ8  
Title : Crystal Structure of the Beta Carbonic Anhydrase psCA3 isolated from Pseudomonas aeruginosa - alternate crystal packing form  
Authors : Pinard, M.A.; Kurian, J.J.; Aggarwal, M.; Agbandje-McKenna, M.; McKenna, R.  
Deposited on : 2016-04-22  
Resolution : 2.58 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

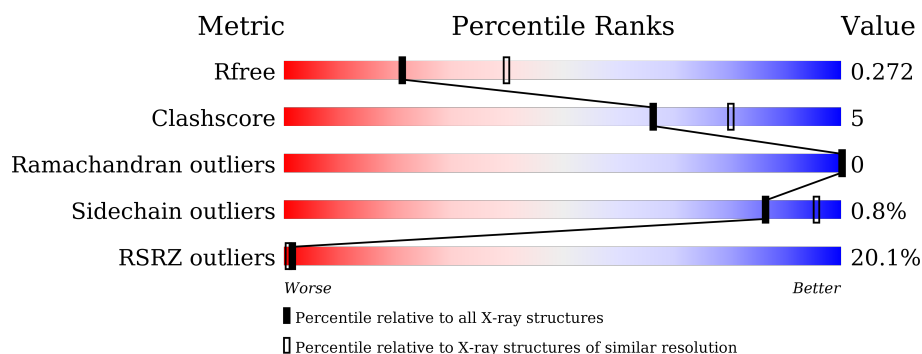
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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))
$R_{free}$	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	215	<div> <div>19%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div> </div>
1	B	215	<div> <div>20%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div></div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3416 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	11	0
			1696	1077	305	307	7			
1	B	209	Total	C	N	O	S	0	11	0
			1696	1077	305	307	7			

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

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

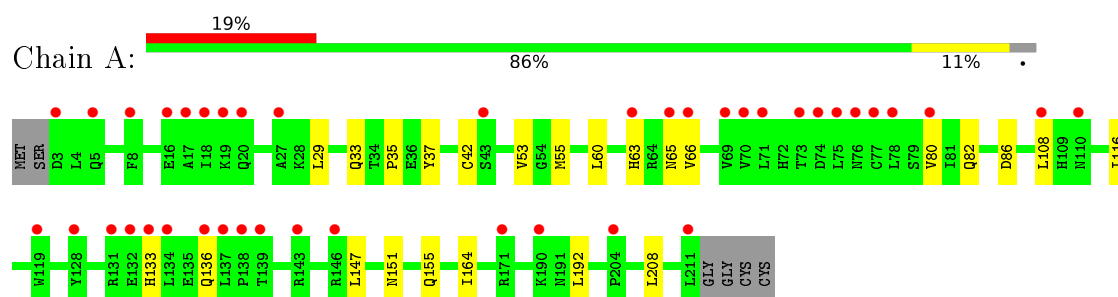
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	9	Total	O	0	0
			9	9		

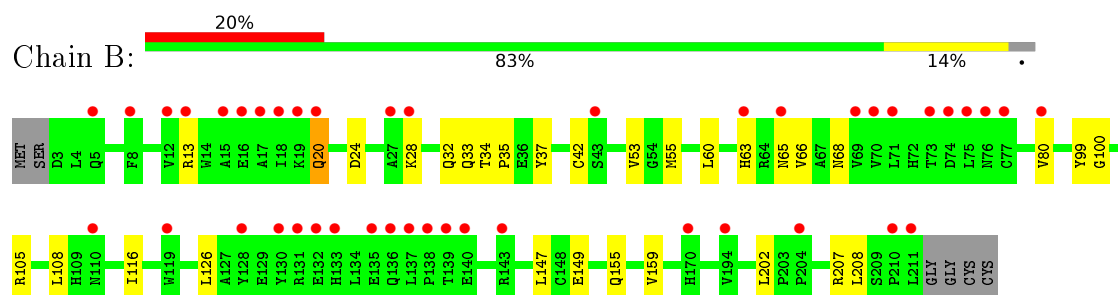
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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



#### • Molecule 1: Carbonic anhydrase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.43Å 69.36Å 77.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.55 – 2.58 35.55 – 2.58	Depositor EDS
% Data completeness (in resolution range)	91.5 (35.55-2.58) 85.3 (35.55-2.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.41 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.212 , 0.275 0.205 , 0.272	Depositor DCC
$R_{free}$ test set	655 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.12 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2979e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.46	0/1778	0.62	0/2419
1	B	0.45	0/1778	0.74	2/2419 (0.1%)
All	All	0.45	0/3556	0.68	2/4838 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	13	ARG	NE-CZ-NH2	13.28	126.94	120.30
1	B	13	ARG	NE-CZ-NH1	-12.63	113.99	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	GLN	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	1696	0	1668	14	0
1	B	1696	0	1668	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	0	1	0
3	B	9	0	0	3	0
All	All	3416	0	3336	33	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 5.

All (33) 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:66:VAL:HG11	1:A:116:ILE:HD11	1.54	0.88
1:B:66:VAL:HG11	1:B:116:ILE:HD11	1.63	0.81
1:B:105[B]:ARG:NH2	3:B:401:HOH:O	2.12	0.80
1:A:55:MET:HG3	1:A:60:LEU:HD13	1.70	0.72
1:B:108:LEU:HD13	1:B:147:LEU:HD22	1.73	0.69
1:B:24:ASP:O	1:B:28:LYS:HG3	1.95	0.67
1:B:63:HIS:HB2	1:B:80:VAL:HG11	1.77	0.66
1:B:53:VAL:HG23	1:B:55:MET:HG2	1.80	0.64
1:A:33:GLN:HG2	1:A:35:PRO:HD3	1.80	0.64
1:A:86:ASP:OD1	3:A:401:HOH:O	2.16	0.61
1:B:55:MET:HG3	1:B:60:LEU:HD13	1.82	0.61
1:A:108:LEU:HD13	1:A:147:LEU:HD22	1.85	0.57
1:A:63:HIS:HB2	1:A:80:VAL:HG11	1.88	0.54
1:A:53:VAL:HG23	1:A:55:MET:HG2	1.90	0.54
1:B:32:GLN:HG3	1:B:34:THR:HG23	1.88	0.54
1:A:151:ASN:O	1:A:155:GLN:HG2	2.11	0.50
1:B:37:TYR:HB2	1:B:60:LEU:HD12	1.95	0.49
1:B:202:LEU:HB2	1:B:207:ARG:HG3	1.95	0.49
1:A:37:TYR:HB2	1:A:60:LEU:HD12	1.96	0.47
1:B:68:ASN:O	1:B:155:GLN:HG3	2.14	0.47
1:B:99:TYR:OH	1:B:149:GLU:OE2	2.28	0.46
1:B:33:GLN:HG2	1:B:35:PRO:HD3	1.97	0.45
1:B:155:GLN:O	1:B:159:VAL:HG23	2.18	0.44
1:A:133:HIS:O	1:A:136:GLN:HB3	2.18	0.43
1:B:42:CYS:HA	1:B:65:ASN:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105[A]:ARG:NH2	3:B:401:HOH:O	2.25	0.43
1:A:192:LEU:HA	1:A:192:LEU:HD23	1.86	0.43
1:A:82:GLN:HB2	1:A:164:ILE:HD13	1.99	0.43
1:A:29:LEU:HD12	1:A:29:LEU:HA	1.88	0.42
1:A:42:CYS:HA	1:A:65:ASN:O	2.19	0.42
1:B:100:GLY:HA2	3:B:401:HOH:O	2.20	0.41
1:B:32:GLN:HG3	1:B:34:THR:CG2	2.51	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	218/215 (101%)	214 (98%)	4 (2%)	0	100	100
1	B	218/215 (101%)	216 (99%)	2 (1%)	0	100	100
All	All	436/430 (101%)	430 (99%)	6 (1%)	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	190/187 (102%)	188 (99%)	2 (1%)	80	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	190/187 (102%)	187 (98%)	3 (2%)	70	88
All	All	380/374 (102%)	375 (99%)	5 (1%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208[A]	LEU
1	A	208[B]	LEU
1	B	20	GLN
1	B	208[A]	LEU
1	B	208[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	10	ASN
1	A	161	HIS
1	B	6	GLN
1	B	10	ASN
1	B	161	HIS

### 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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	209/215 (97%)	0.96	41 (19%)  	30, 49, 77, 105	0
1	B	209/215 (97%)	0.99	43 (20%)  	30, 49, 76, 103	0
All	All	418/430 (97%)	0.98	84 (20%)  	30, 49, 77, 105	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	GLU	5.5
1	B	20	GLN	5.3
1	A	211	LEU	5.2
1	A	18	ILE	5.0
1	A	132	GLU	5.0
1	A	134	LEU	4.7
1	A	20	GLN	4.2
1	B	18	ILE	3.8
1	B	77	CYS	3.7
1	B	73	THR	3.7
1	B	12	VAL	3.6
1	A	133	HIS	3.6
1	A	137	LEU	3.6
1	B	8	PHE	3.5
1	B	204	PRO	3.5
1	A	73	THR	3.5
1	A	77	CYS	3.5
1	B	128	TYR	3.5
1	A	204	PRO	3.4
1	B	137	LEU	3.4
1	A	16	GLU	3.3
1	A	128	TYR	3.3
1	B	210	PRO	3.3
1	B	76	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	5	GLN	3.2
1	B	170	HIS	3.2
1	B	119	TRP	3.1
1	B	143	ARG	3.0
1	A	119	TRP	3.0
1	B	140[A]	GLU	2.9
1	A	138	PRO	2.9
1	B	75	LEU	2.9
1	A	136	GLN	2.7
1	B	16	GLU	2.7
1	B	139	THR	2.7
1	A	110[A]	ASN	2.7
1	A	143	ARG	2.7
1	B	136	GLN	2.7
1	B	135	GLU	2.7
1	B	63	HIS	2.7
1	A	76	ASN	2.6
1	A	74	ASP	2.6
1	B	65	ASN	2.5
1	A	108	LEU	2.5
1	A	65	ASN	2.5
1	A	63	HIS	2.5
1	B	133	HIS	2.5
1	B	211	LEU	2.5
1	B	131	ARG	2.5
1	A	19	LYS	2.4
1	A	3	ASP	2.4
1	A	27	ALA	2.4
1	B	15	ALA	2.4
1	A	8	PHE	2.4
1	A	69	VAL	2.4
1	B	74	ASP	2.4
1	A	75	LEU	2.4
1	B	28	LYS	2.4
1	A	43	SER	2.4
1	A	71	LEU	2.4
1	A	70	VAL	2.3
1	B	80	VAL	2.3
1	B	110[A]	ASN	2.3
1	B	70	VAL	2.3
1	B	194	VAL	2.3
1	B	138	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	19	LYS	2.2
1	B	71	LEU	2.2
1	A	5	GLN	2.2
1	B	130	TYR	2.2
1	A	66	VAL	2.2
1	A	131	ARG	2.2
1	A	171	ARG	2.2
1	A	139	THR	2.2
1	A	80	VAL	2.1
1	B	27	ALA	2.1
1	B	13	ARG	2.1
1	A	17	ALA	2.1
1	A	78	LEU	2.1
1	A	146	ARG	2.1
1	B	43	SER	2.1
1	A	190	LYS	2.1
1	B	17	ALA	2.1
1	B	69	VAL	2.0

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	301	1/1	0.98	0.20	0.54	46,46,46,46	0
2	ZN	B	301	1/1	0.99	0.17	-0.10	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.