



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:42 pm BST

PDB ID : 1I6O
Title : CRYSTAL STRUCTURE OF E. COLI BETA CARBONIC ANHYDRASE (ECCA)
Authors : Cronk, J.D.; Endrizzi, J.A.; Cronk, M.R.; O'Neill, J.W.; Zhang, K.Y.J.
Deposited on : 2001-03-02
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

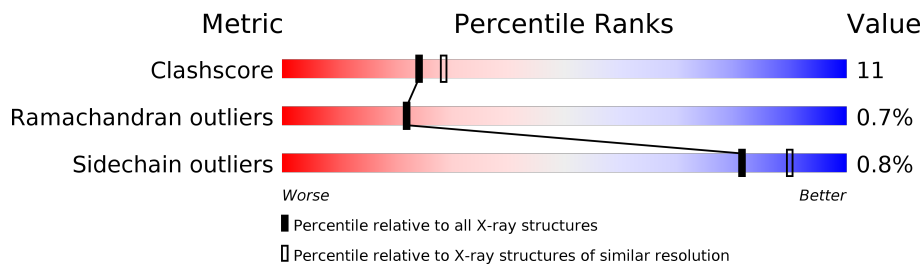
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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)

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	220	
1	B	220	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3510 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
			Total	C	N	O	S	Se			
1	A	213	1706	1081	304	312	5	4	0	0	0
1	B	214	1715	1087	306	313	5	4	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P61517
A	17	MSE	MET	MODIFIED RESIDUE	UNP P61517
A	137	MSE	MET	MODIFIED RESIDUE	UNP P61517
A	152	MSE	MET	MODIFIED RESIDUE	UNP P61517
A	164	MSE	MET	MODIFIED RESIDUE	UNP P61517
B	1	MSE	MET	MODIFIED RESIDUE	UNP P61517
B	17	MSE	MET	MODIFIED RESIDUE	UNP P61517
B	137	MSE	MET	MODIFIED RESIDUE	UNP P61517
B	152	MSE	MET	MODIFIED RESIDUE	UNP P61517
B	164	MSE	MET	MODIFIED RESIDUE	UNP P61517

- 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	50	Total	O	0	0
			50	50		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	37	Total	O	0	0
			37	37		

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	81.24Å 81.24Å 162.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.20	Depositor
% Data completeness (in resolution range)	99.3 (39.36-2.20)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3510	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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

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	0.33	0/1739	0.57	1/2353 (0.0%)
1	B	0.29	0/1748	0.55	0/2364
All	All	0.31	0/3487	0.56	1/4717 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	PHE	N-CA-C	-5.02	97.44	111.00

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	1706	0	1686	45	0
1	B	1715	0	1699	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	50	0	0	0	0
3	B	37	0	0	0	0
All	All	3510	0	3385	75	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 11.

All (75) 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:B:204:ARG:HA	1:B:204:ARG:HE	1.40	0.86
1:A:133:LEU:HD13	1:A:213:LYS:HG2	1.62	0.79
1:A:6:THR:HG22	1:A:10:ASN:HD21	1.48	0.78
1:A:141:ARG:NE	1:A:141:ARG:HA	2.00	0.76
1:B:138:PRO:HB2	1:B:140:GLU:OE2	1.92	0.69
1:A:152:MSE:HE1	1:A:208:GLY:C	2.14	0.68
1:B:31:GLN:HB2	1:B:33:GLN:HE21	1.61	0.66
1:B:152:MSE:HE1	1:B:208:GLY:C	2.18	0.64
1:A:36:ARG:NE	1:A:36:ARG:HA	2.13	0.62
1:A:15:SER:O	1:A:19:VAL:HG23	1.99	0.62
1:A:150:ASN:O	1:A:154:GLN:HG2	1.99	0.61
1:B:133:LEU:HD13	1:B:213:LYS:HA	1.83	0.60
1:A:57:PRO:HB3	1:B:48:PRO:HD3	1.84	0.60
1:B:36:ARG:NE	1:B:36:ARG:HA	2.17	0.60
1:B:37:PHE:HB2	1:B:60:LEU:HD23	1.85	0.59
1:A:6:THR:HG22	1:A:10:ASN:ND2	2.18	0.56
1:A:141:ARG:CA	1:A:141:ARG:NE	2.71	0.54
1:A:12:ALA:O	1:A:16:LYS:HG2	2.09	0.53
1:A:139:GLN:HA	1:A:142:ARG:HD2	1.91	0.52
1:B:82:GLN:HB2	1:B:163:ILE:HD13	1.92	0.51
1:B:127:TRP:CE3	1:B:134:LEU:HD13	2.46	0.51
1:A:127:TRP:CE3	1:A:146:LEU:HD22	2.46	0.51
1:A:28:LYS:HA	1:A:31:GLN:NE2	2.26	0.51
1:A:176:ILE:HD11	1:A:201:LEU:HD13	1.91	0.50
1:A:177:HIS:CE1	1:B:4:ILE:HG13	2.46	0.50
1:B:204:ARG:HA	1:B:204:ARG:NE	2.19	0.50
1:B:111:PRO:HG2	1:B:113:LEU:HG	1.93	0.50
1:A:67:ALA:CB	1:A:123:ILE:HD11	2.42	0.49
1:B:166:SER:O	1:B:170:ARG:HG3	2.11	0.49
1:B:24:GLY:O	1:B:28:LYS:HG3	2.13	0.48
1:B:19:VAL:HG13	1:B:20:GLU:HG3	1.95	0.48
1:B:204:ARG:HH21	1:B:207:HIS:HB3	1.77	0.48
1:B:16:LYS:O	1:B:19:VAL:HG12	2.15	0.47
1:B:63:HIS:HB2	1:B:80:VAL:HG11	1.97	0.47
1:A:37:PHE:HB2	1:A:60:LEU:HD23	1.96	0.47
1:B:152:MSE:HE3	1:B:193:VAL:CG1	2.45	0.47
1:A:141:ARG:HE	1:A:141:ARG:HA	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:HA	1:A:142:ARG:CD	2.46	0.45
1:A:134:LEU:O	1:A:137:MSE:HB3	2.16	0.45
1:A:46:ARG:O	1:B:57:PRO:HB2	2.17	0.45
1:A:57:PRO:HB3	1:B:48:PRO:CD	2.46	0.45
1:A:165:GLN:NE2	1:A:198:ARG:HG2	2.32	0.44
1:A:212:LEU:C	1:A:214:LEU:H	2.20	0.44
1:A:215:LYS:HG2	1:A:215:LYS:O	2.17	0.44
1:A:7:LEU:CD2	1:B:55:LEU:HD21	2.48	0.44
1:A:30:ALA:O	1:A:32:ALA:N	2.50	0.44
1:B:47:VAL:HG12	1:B:52:LEU:HG	2.00	0.44
1:A:183:ILE:HG13	1:B:29:LEU:HB3	2.00	0.44
1:B:127:TRP:CE3	1:B:146:LEU:HD22	2.53	0.44
1:A:132:SER:O	1:A:136:GLU:HG2	2.18	0.44
1:A:36:ARG:NE	1:A:36:ARG:CA	2.80	0.44
1:B:66:VAL:O	1:B:67:ALA:HB3	2.18	0.44
1:A:7:LEU:HD21	1:B:55:LEU:HD21	1.99	0.43
1:B:141:ARG:NH2	1:B:144:ASP:OD2	2.51	0.43
1:A:141:ARG:NH1	1:A:144:ASP:OD1	2.52	0.43
1:B:192:ASP:O	1:B:192:ASP:CG	2.56	0.43
1:A:50:GLU:H	1:A:50:GLU:CD	2.23	0.42
1:A:82:GLN:HG3	1:B:115:LEU:HB3	2.02	0.42
1:B:24:GLY:HA2	1:B:27:GLU:OE1	2.20	0.42
1:A:34:LYS:HA	1:A:35:PRO:HD3	1.95	0.42
1:A:55:LEU:HD23	1:B:2:LYS:HD2	2.01	0.42
1:A:141:ARG:CA	1:A:141:ARG:HE	2.33	0.41
1:B:41:GLY:O	1:B:64:ARG:HA	2.20	0.41
1:A:106:ALA:O	1:A:111:PRO:HD2	2.21	0.41
1:A:177:HIS:NE2	1:B:4:ILE:HG13	2.35	0.41
1:A:151:VAL:O	1:A:155:VAL:HG23	2.21	0.41
1:B:199:GLU:CD	1:B:199:GLU:N	2.74	0.41
1:B:138:PRO:HG2	1:B:141:ARG:HB2	2.03	0.41
1:B:36:ARG:NE	1:B:36:ARG:CA	2.84	0.41
1:A:164:MSE:HE1	1:A:174:VAL:HB	2.02	0.40
1:A:24:GLY:HA2	1:A:27:GLU:HG3	2.03	0.40
1:B:156:TYR:OH	1:B:202:GLU:OE1	2.38	0.40
1:A:55:LEU:CD2	1:B:2:LYS:HD2	2.52	0.40
1:B:56:GLU:HB3	1:B:57:PRO:HD2	2.01	0.40
1:A:56:GLU:HB2	1:A:59:GLU:OE2	2.20	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	211/220 (96%)	198 (94%)	11 (5%)	2 (1%)	17	16
1	B	212/220 (96%)	196 (92%)	15 (7%)	1 (0%)	29	31
All	All	423/440 (96%)	394 (93%)	26 (6%)	3 (1%)	22	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ALA
1	A	31	GLN
1	B	192	ASP

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	186/187 (100%)	185 (100%)	1 (0%)	88	94
1	B	187/187 (100%)	185 (99%)	2 (1%)	73	85
All	All	373/374 (100%)	370 (99%)	3 (1%)	81	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	B	140	GLU
1	B	204	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	31	GLN
1	A	110	ASN
1	B	33	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 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

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.