wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 10:41 PM EST

PDB ID	:	1G5C
Title	:	CRYSTAL STRUCTURE OF THE 'CAB' TYPE BETA CLASS CARBONIC ANHYDRASE FROM METHANOBACTERIUM THERMOAUTOTROPHICUM
Authors	:	Strop, P.; Smith, K.S.; Iverson, T.M.; Ferry, J.G.; Rees, D.C.
Deposited on	:	2000-10-31
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

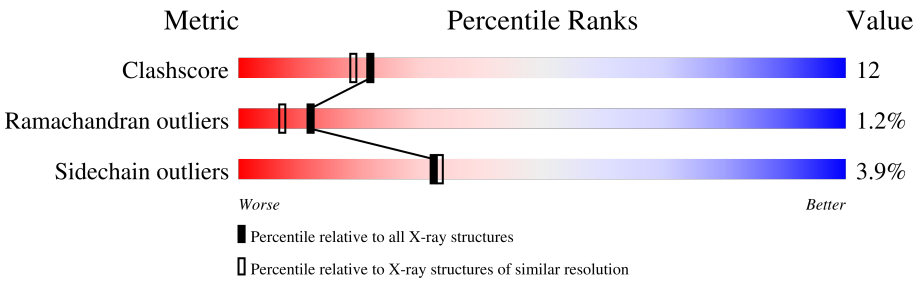
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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	170	75% 22% • • •
1	B	170	71% 22% • 7%
1	C	170	75% 21% • •
1	D	170	71% 22% • 7%
1	E	170	77% 19% • •
1	F	170	66% 25% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8010 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 BETA-CARBONIC ANHYDRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	169	1311	820	228	257	6	61	0	0
1	B	158	1210	755	208	241	6	31	0	0
1	C	169	1311	820	228	257	6	78	0	0
1	D	158	1210	755	208	241	6	59	0	0
1	E	169	1311	820	228	257	6	151	0	0
1	F	155	1187	743	204	234	6	42	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ASP	VAL	conflict	UNP Q50565
B	79	ASP	VAL	conflict	UNP Q50565
C	79	ASP	VAL	conflict	UNP Q50565
D	79	ASP	VAL	conflict	UNP Q50565
E	79	ASP	VAL	conflict	UNP Q50565
F	79	ASP	VAL	conflict	UNP Q50565

- 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
2	B	1	1	1	0	0
2	C	1	1	1	0	0

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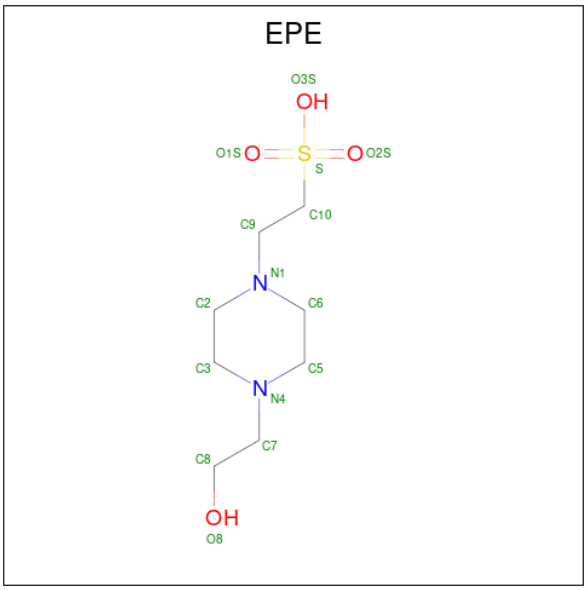
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 15 8 2 4 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	C	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
4	E	1	15	8	2	4	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	83	83	83	0	0
			Total	O		
5	B	73	73	73	0	0
			Total	O		
5	C	58	58	58	0	0
			Total	O		
5	D	49	49	49	0	0
			Total	O		
5	E	84	84	84	0	0
			Total	O		
5	F	66	66	66	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.

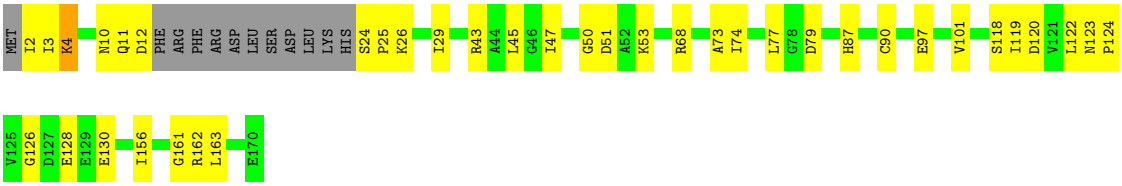
Note EDS was not executed.

• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain A:

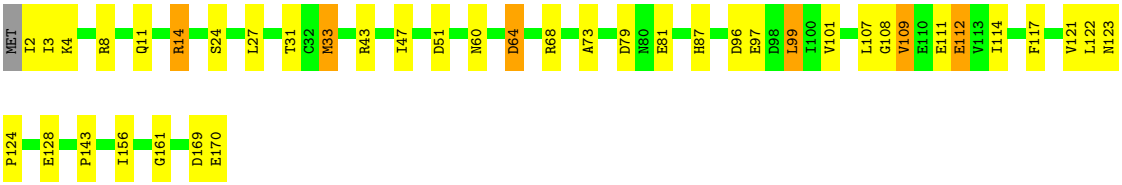
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain B:



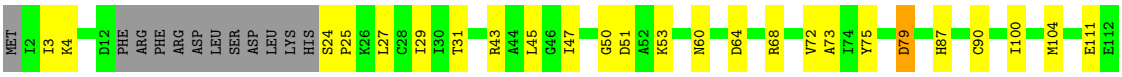
• Molecule 1: BETA-CARBONIC ANHYDRASE

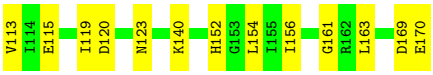
Chain C:



• Molecule 1: BETA-CARBONIC ANHYDRASE

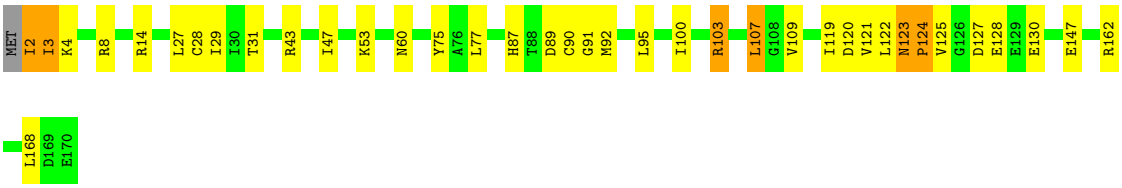
Chain D:





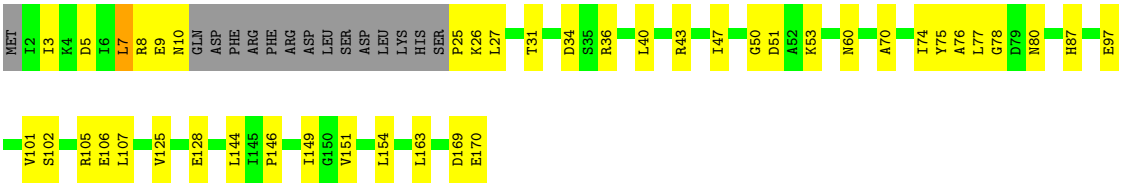
• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain E:



• Molecule 1: BETA-CARBONIC ANHYDRASE

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.67Å 113.21Å 156.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.10	Depositor
% Data completeness (in resolution range)	98.8 (18.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8010	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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: CA, EPE, 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	3.39	1/1323 (0.1%)	0.67	1/1783 (0.1%)
1	B	0.39	0/1218	0.64	0/1642
1	C	0.36	0/1323	0.66	1/1783 (0.1%)
1	D	0.34	0/1218	0.62	0/1642
1	E	0.45	0/1323	0.73	0/1783
1	F	0.37	0/1195	0.66	0/1610
All	All	1.46	1/7600 (0.0%)	0.66	2/10243 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	GLU	C-OXT	122.24	3.55	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	33	MET	CG-SD-CE	6.71	110.94	100.20
1	A	27	LEU	CA-CB-CG	5.31	127.52	115.30

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	1311	0	1341	32	0
1	B	1210	0	1241	39	0
1	C	1311	0	1341	31	0
1	D	1210	0	1241	30	0
1	E	1311	0	1341	27	0
1	F	1187	0	1225	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	15	0	17	3	0
4	C	15	0	17	0	0
4	E	15	0	17	4	0
5	A	83	0	0	2	0
5	B	73	0	0	1	0
5	C	58	0	0	4	0
5	D	49	0	0	0	0
5	E	84	0	0	0	0
5	F	66	0	0	1	0
All	All	8010	0	7781	172	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 12.

The worst 5 of 172 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:D:24:SER:HB2	1:D:25:PRO:HD3	1.44	0.97
1:A:118:SER:HA	1:A:122:LEU:HD23	1.50	0.94
1:C:8:ARG:O	1:C:11:GLN:HG2	1.70	0.90
1:E:2:ILE:HD12	1:E:3:ILE:HD12	1.58	0.85
1:C:73:ALA:HB1	1:C:79:ASP:OD1	1.76	0.85

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	167/170 (98%)	157 (94%)	7 (4%)	3 (2%)	8 4
1	B	154/170 (91%)	152 (99%)	2 (1%)	0	100 100
1	C	167/170 (98%)	154 (92%)	10 (6%)	3 (2%)	8 4
1	D	154/170 (91%)	146 (95%)	8 (5%)	0	100 100
1	E	167/170 (98%)	158 (95%)	4 (2%)	5 (3%)	4 1
1	F	151/170 (89%)	142 (94%)	8 (5%)	1 (1%)	22 18
All	All	960/1020 (94%)	909 (95%)	39 (4%)	12 (1%)	12 7

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	VAL
1	C	109	VAL
1	C	123	ASN
1	E	121	VAL
1	A	94	ARG

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	147/148 (99%)	143 (97%)	4 (3%)	44 48
1	B	136/148 (92%)	132 (97%)	4 (3%)	42 46
1	C	147/148 (99%)	141 (96%)	6 (4%)	30 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	136/148 (92%)	132 (97%)	4 (3%)	42	46
1	E	147/148 (99%)	138 (94%)	9 (6%)	18	16
1	F	133/148 (90%)	127 (96%)	6 (4%)	27	27
All	All	846/888 (95%)	813 (96%)	33 (4%)	32	33

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	9	GLU
1	F	27	LEU
1	F	77	LEU
1	C	99	LEU
1	C	64	ASP

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

Mol	Chain	Res	Type
1	B	123	ASN
1	D	123	ASN
1	E	123	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 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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	EPE	C	2202	-	15,15,15	1.21	1 (6%)	18,20,20	1.17	1 (5%)
4	EPE	A	2201	-	15,15,15	1.47	4 (26%)	18,20,20	1.07	1 (5%)
4	EPE	E	2203	-	15,15,15	1.75	4 (26%)	18,20,20	2.40	6 (33%)

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	EPE	C	2202	-	-	2/9/19/19	0/1/1/1
4	EPE	A	2201	-	-	2/9/19/19	0/1/1/1
4	EPE	E	2203	-	-	3/9/19/19	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2203	EPE	C6-N1	4.45	1.59	1.46
4	A	2201	EPE	C9-N1	2.90	1.54	1.47
4	E	2203	EPE	C7-C8	-2.69	1.40	1.51
4	E	2203	EPE	C2-N1	2.58	1.54	1.46
4	A	2201	EPE	C2-N1	2.47	1.53	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2203	EPE	C5-N4-C3	5.67	121.59	108.83
4	E	2203	EPE	C3-C2-N1	-4.88	100.64	110.64
4	C	2202	EPE	O1S-S-C10	-3.10	103.18	106.92
4	E	2203	EPE	O8-C8-C7	-2.98	98.83	111.19
4	E	2203	EPE	C7-N4-C3	2.75	118.27	111.23

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2201	EPE	C10-C9-N1-C2
4	E	2203	EPE	C10-C9-N1-C6
4	E	2203	EPE	C8-C7-N4-C3
4	C	2202	EPE	C10-C9-N1-C2
4	C	2202	EPE	C10-C9-N1-C6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2201	EPE	3	0
4	E	2203	EPE	4	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.