



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 03:40 PM EDT

PDB ID : 3E3I
Title : H. influenzae beta-carbonic anhydrase, variant G41A with 100 mM bicarbonate
Authors : Rowlett, R.S.; Failing, H.
Deposited on : 2008-08-07
Resolution : 2.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

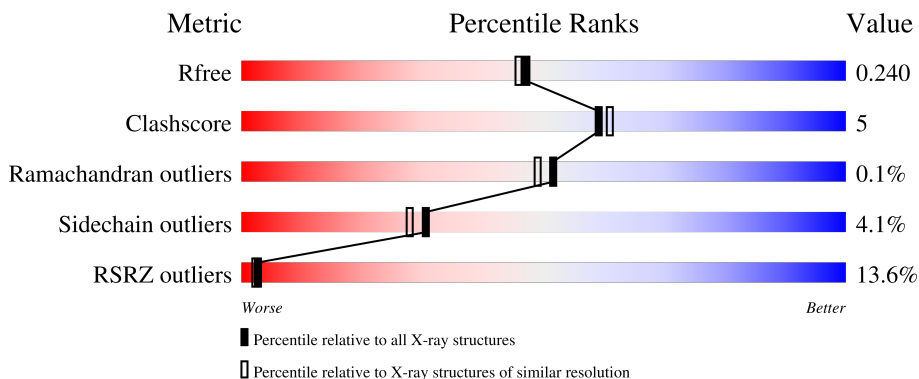
1 Overall quality at a glance

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.



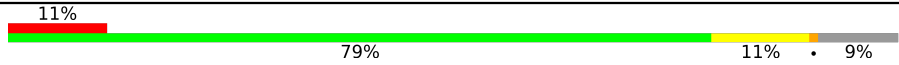

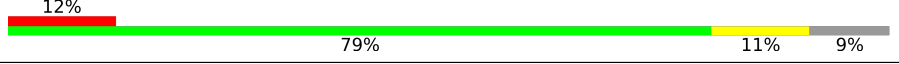
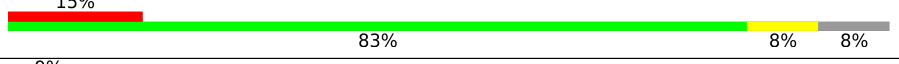

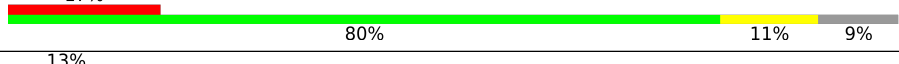

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 $\leq 5\%$. 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	229	 9% 75% 14% • 9%
1	B	229	 11% 80% 11% • 7%
1	C	229	 9% 77% 12% • 9%
1	D	229	 13% 83% 10% • 7%
1	E	229	 16% 80% 12% • 7%

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Mol	Chain	Length	Quality of chain
1	F	229	
1	G	229	
1	H	229	
1	I	229	
1	J	229	
1	K	229	
1	L	229	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCT	B	233	-	-	X	-
4	BCT	C	232	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21039 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	Total 1683	C 1069	N 300	O 305	S 9	0	2	0
1	B	212	Total 1711	C 1087	N 304	O 311	S 9	0	1	0
1	C	208	Total 1681	C 1067	N 300	O 305	S 9	0	1	0
1	D	213	Total 1722	C 1094	N 306	O 313	S 9	0	1	0
1	E	212	Total 1714	C 1088	N 305	O 312	S 9	0	1	0
1	F	208	Total 1680	C 1070	N 300	O 301	S 9	0	1	0
1	G	214	Total 1716	C 1090	N 305	O 312	S 9	0	0	0
1	H	209	Total 1693	C 1075	N 302	O 307	S 9	0	1	0
1	I	210	Total 1696	C 1078	N 302	O 307	S 9	0	1	0
1	J	205	Total 1669	C 1063	N 300	O 297	S 9	0	2	0
1	K	209	Total 1693	C 1075	N 302	O 307	S 9	0	1	0
1	L	206	Total 1656	C 1052	N 297	O 298	S 9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	GLY	engineered mutation	UNP P45148
B	41	ALA	GLY	engineered mutation	UNP P45148
C	41	ALA	GLY	engineered mutation	UNP P45148
D	41	ALA	GLY	engineered mutation	UNP P45148
E	41	ALA	GLY	engineered mutation	UNP P45148

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Chain	Residue	Modelled	Actual	Comment	Reference
F	41	ALA	GLY	engineered mutation	UNP P45148
G	41	ALA	GLY	engineered mutation	UNP P45148
H	41	ALA	GLY	engineered mutation	UNP P45148
I	41	ALA	GLY	engineered mutation	UNP P45148
J	41	ALA	GLY	engineered mutation	UNP P45148
K	41	ALA	GLY	engineered mutation	UNP P45148
L	41	ALA	GLY	engineered mutation	UNP P45148

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

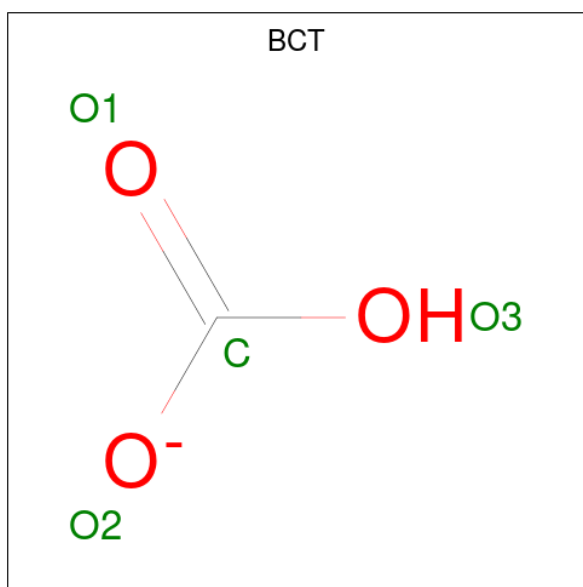
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 1 3	0	0
4	C	1	Total C O 4 1 3	0	0
4	D	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0
4	G	1	Total C O 4 1 3	0	0
4	H	1	Total C O 4 1 3	0	0
4	I	1	Total C O 4 1 3	0	0
4	J	1	Total C O 4 1 3	0	0
4	K	1	Total C O 4 1 3	0	0
4	L	1	Total C O 4 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	49	Total O 49 49	0	0

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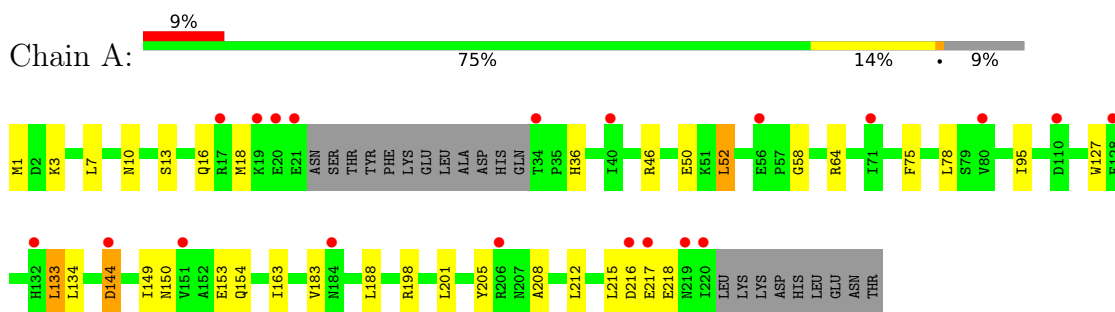
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	59	Total O 59 59	0	0
5	C	43	Total O 43 43	0	0
5	D	53	Total O 53 53	0	0
5	E	65	Total O 65 65	0	0
5	F	56	Total O 56 56	0	0
5	G	54	Total O 54 54	0	0
5	H	50	Total O 50 50	0	0
5	I	46	Total O 46 46	0	0
5	J	43	Total O 43 43	0	0
5	K	44	Total O 44 44	0	0
5	L	42	Total O 42 42	0	0

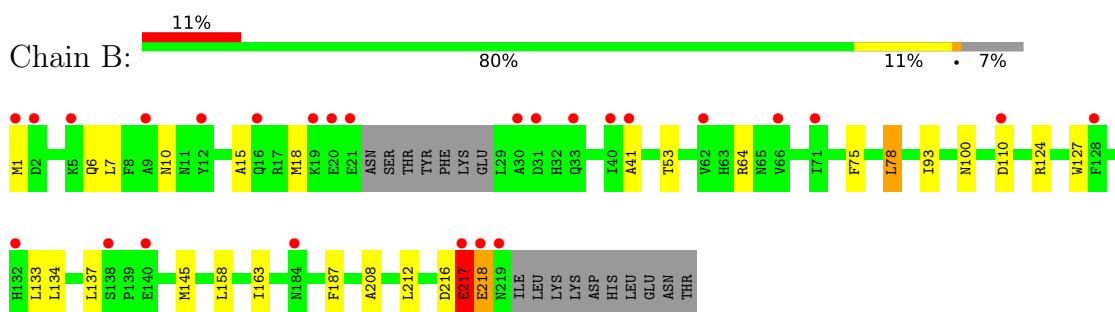
3 Residue-property plots [i](#)

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.

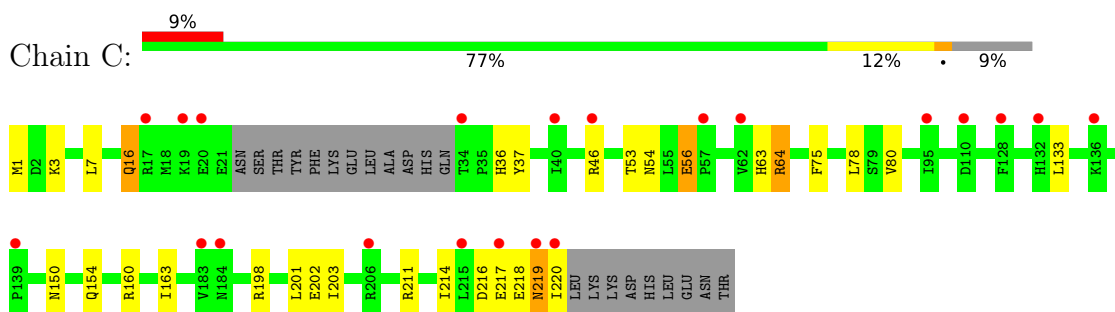
- Molecule 1: Carbonic anhydrase 2



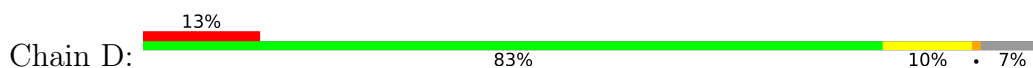
- Molecule 1: Carbonic anhydrase 2

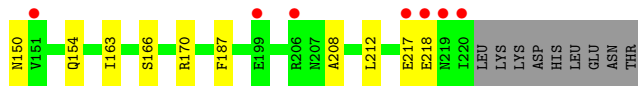
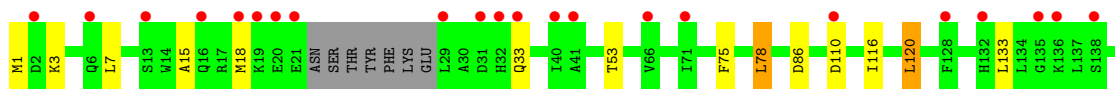


- Molecule 1: Carbonic anhydrase 2

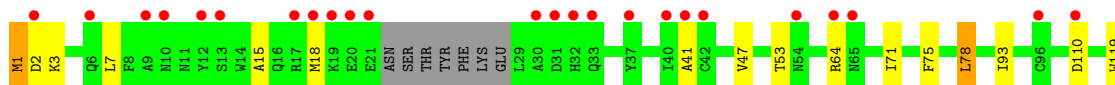
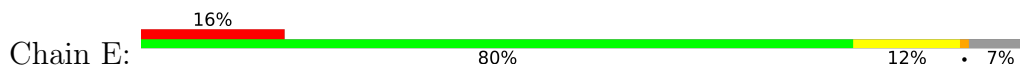


- Molecule 1: Carbonic anhydrase 2

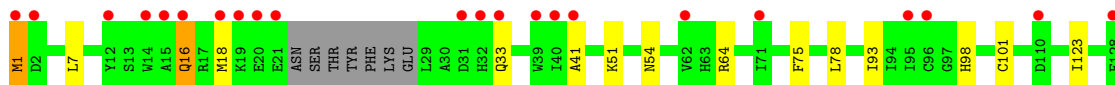
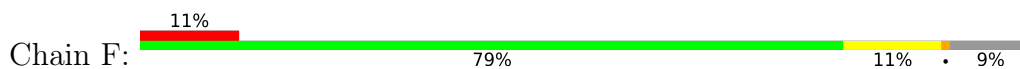




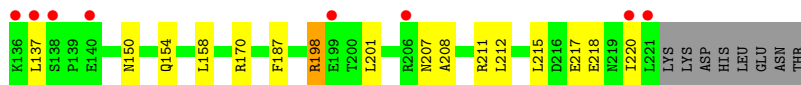
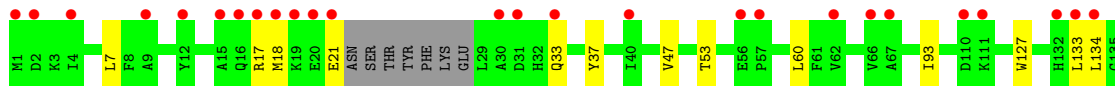
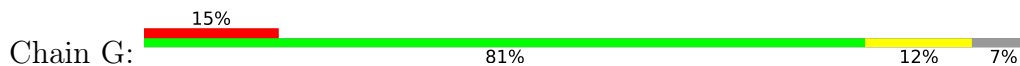
- Molecule 1: Carbonic anhydrase 2



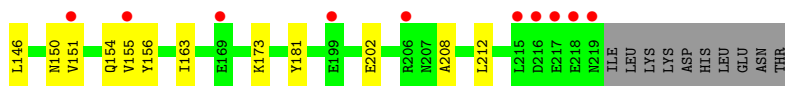
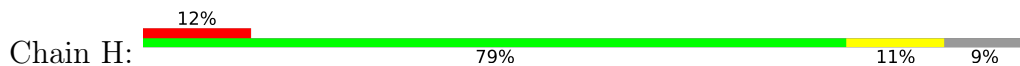
- Molecule 1: Carbonic anhydrase 2



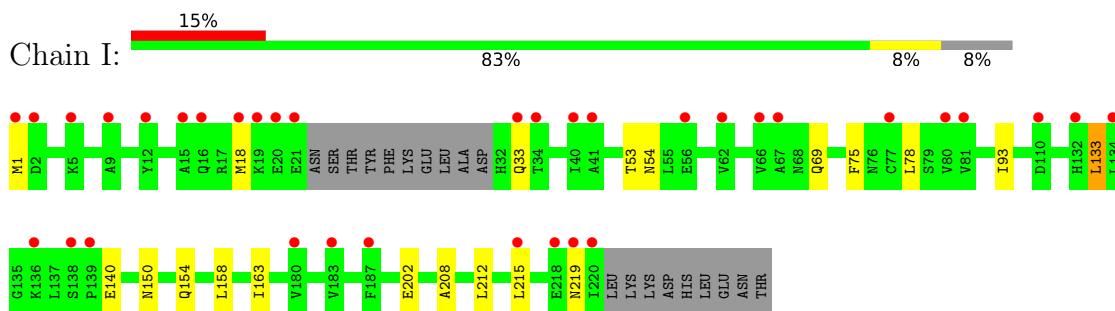
- Molecule 1: Carbonic anhydrase 2



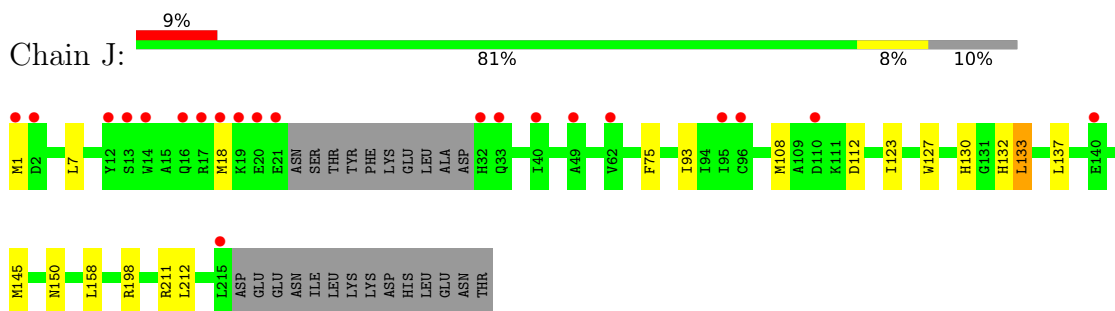
- Molecule 1: Carbonic anhydrase 2



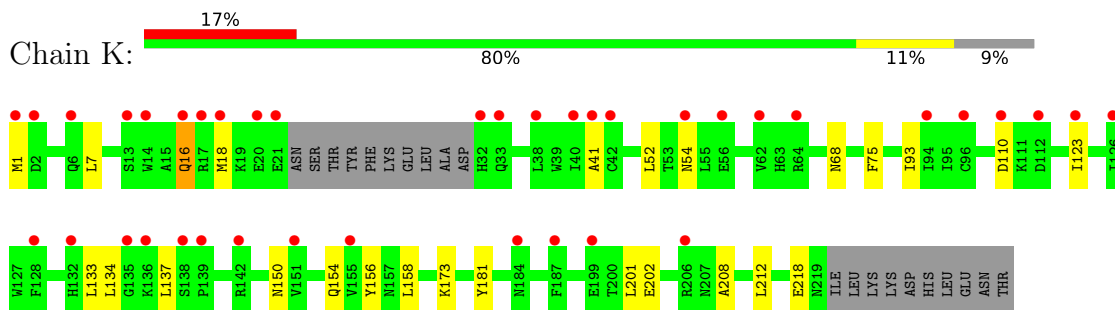
- Molecule 1: Carbonic anhydrase 2



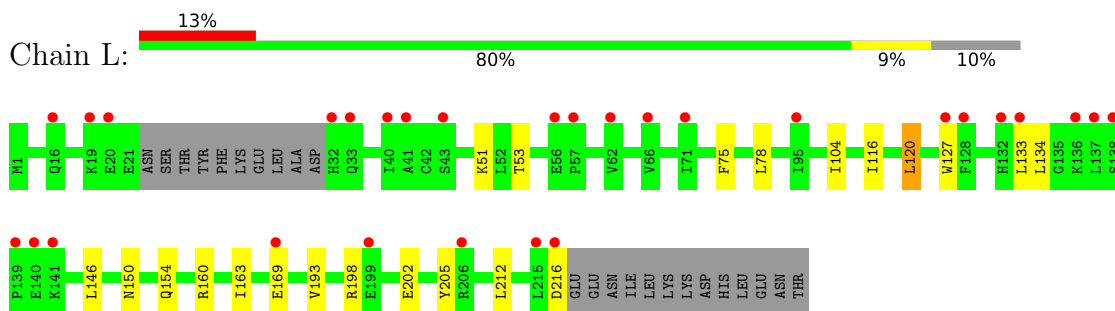
- Molecule 1: Carbonic anhydrase 2



- Molecule 1: Carbonic anhydrase 2



- Molecule 1: Carbonic anhydrase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.59Å 144.44Å 104.89Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	29.75 – 2.00 29.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (29.75-2.00) 89.6 (29.75-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.00Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.236 0.207 , 0.240	Depositor DCC
R_{free} test set	10347 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21039	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.84 % 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 5.9966e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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, BCT, SO4

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	0.54	0/1725	0.66	2/2336 (0.1%)
1	B	0.51	0/1751	0.62	0/2371
1	C	0.52	0/1717	0.67	3/2325 (0.1%)
1	D	0.50	0/1759	0.59	0/2382
1	E	0.56	0/1751	0.64	0/2371
1	F	0.54	0/1717	0.63	1/2325 (0.0%)
1	G	0.57	0/1752	0.65	2/2373 (0.1%)
1	H	0.53	0/1730	0.62	0/2342
1	I	0.52	0/1733	0.58	0/2346
1	J	0.49	0/1707	0.59	0/2311
1	K	0.50	0/1730	0.59	0/2342
1	L	0.48	0/1692	0.62	1/2291 (0.0%)
All	All	0.52	0/20764	0.62	9/28115 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	LEU	CA-CB-CG	8.34	134.47	115.30
1	G	170	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	F	160	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	C	64	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	64	ARG	NE-CZ-NH2	-6.16	117.22	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1683	0	1672	29	0
1	B	1711	0	1692	16	0
1	C	1681	0	1665	36	0
1	D	1722	0	1702	15	0
1	E	1714	0	1691	18	0
1	F	1680	0	1669	17	0
1	G	1716	0	1701	18	0
1	H	1693	0	1671	18	0
1	I	1696	0	1671	17	0
1	J	1669	0	1655	11	0
1	K	1693	0	1671	14	0
1	L	1656	0	1645	10	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
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	H	10	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	B	4	0	0	2	0
4	C	4	0	0	3	0
4	D	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	4	0	0	1	0
4	F	4	0	0	0	0
4	G	4	0	0	1	0
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	1	0
4	L	4	0	0	0	0
5	A	49	0	0	1	0
5	B	59	0	0	0	0
5	C	43	0	0	3	0
5	D	53	0	0	0	0
5	E	65	0	0	0	0
5	F	56	0	0	0	0
5	G	54	0	0	0	0
5	H	50	0	0	0	0
5	I	46	0	0	1	0
5	J	43	0	0	1	0
5	K	44	0	0	0	0
5	L	42	0	0	0	0
All	All	21039	0	20105	189	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.

The worst 5 of 189 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:I:133:LEU:HD21	1:I:215:LEU:HD21	1.34	1.09
1:C:203:ILE:HD12	1:F:214:ILE:HD11	1.37	1.04
1:C:214:ILE:HD11	1:F:203:ILE:HD12	1.35	1.03
1:H:78:LEU:HD12	1:H:163:ILE:HD12	1.43	1.00
1:B:53:THR:HG22	1:D:7:LEU:HD21	1.46	0.97

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	206/229 (90%)	200 (97%)	5 (2%)	1 (0%)	29	23
1	B	209/229 (91%)	203 (97%)	5 (2%)	1 (0%)	29	23
1	C	205/229 (90%)	200 (98%)	5 (2%)	0	100	100
1	D	210/229 (92%)	205 (98%)	5 (2%)	0	100	100
1	E	209/229 (91%)	204 (98%)	5 (2%)	0	100	100
1	F	205/229 (90%)	201 (98%)	4 (2%)	0	100	100
1	G	210/229 (92%)	204 (97%)	6 (3%)	0	100	100
1	H	206/229 (90%)	201 (98%)	5 (2%)	0	100	100
1	I	207/229 (90%)	199 (96%)	7 (3%)	1 (0%)	29	23
1	J	203/229 (89%)	196 (97%)	7 (3%)	0	100	100
1	K	206/229 (90%)	202 (98%)	4 (2%)	0	100	100
1	L	202/229 (88%)	199 (98%)	3 (2%)	0	100	100
All	All	2478/2748 (90%)	2414 (97%)	61 (2%)	3 (0%)	51	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	GLU
1	B	217	GLU
1	I	219	ASN

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	183/201 (91%)	177 (97%)	6 (3%)	38	37
1	B	185/201 (92%)	176 (95%)	9 (5%)	25	21
1	C	182/201 (90%)	175 (96%)	7 (4%)	33	31
1	D	186/201 (92%)	178 (96%)	8 (4%)	29	26
1	E	185/201 (92%)	176 (95%)	9 (5%)	25	21
1	F	181/201 (90%)	170 (94%)	11 (6%)	18	14
1	G	185/201 (92%)	180 (97%)	5 (3%)	44	46
1	H	183/201 (91%)	178 (97%)	5 (3%)	44	46
1	I	182/201 (90%)	176 (97%)	6 (3%)	38	37
1	J	180/201 (90%)	172 (96%)	8 (4%)	28	25
1	K	183/201 (91%)	174 (95%)	9 (5%)	25	21
1	L	179/201 (89%)	173 (97%)	6 (3%)	37	36
All	All	2194/2412 (91%)	2105 (96%)	89 (4%)	30	28

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	54	ASN
1	J	198	ARG
1	H	120	LEU
1	I	202	GLU
1	K	16	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	54	ASN
1	I	16	GLN
1	L	54	ASN
1	H	54	ASN
1	I	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	BCT	L	232	-	2,3,3	0.60	0	2,3,3	0.13	0
4	BCT	K	232	-	2,3,3	0.66	0	2,3,3	0.27	0
3	SO4	A	231	-	4,4,4	0.21	0	6,6,6	0.27	0
3	SO4	C	231	-	4,4,4	0.18	0	6,6,6	0.31	0
3	SO4	B	232	-	4,4,4	0.23	0	6,6,6	0.31	0
3	SO4	J	231	-	4,4,4	0.18	0	6,6,6	0.42	0
3	SO4	H	231	-	4,4,4	0.17	0	6,6,6	0.47	0
4	BCT	B	233	-	2,3,3	0.62	0	2,3,3	0.30	0
3	SO4	L	231	-	4,4,4	0.17	0	6,6,6	0.38	0
3	SO4	D	231	-	4,4,4	0.20	0	6,6,6	0.43	0
3	SO4	B	231	-	4,4,4	0.19	0	6,6,6	0.34	0
3	SO4	H	232	-	4,4,4	0.16	0	6,6,6	0.36	0
4	BCT	I	232	-	2,3,3	0.73	0	2,3,3	0.46	0
4	BCT	D	232	-	2,3,3	0.66	0	2,3,3	0.46	0
3	SO4	E	232	-	4,4,4	0.17	0	6,6,6	0.53	0
4	BCT	J	232	-	2,3,3	0.68	0	2,3,3	0.36	0
4	BCT	F	231	-	2,3,3	0.57	0	2,3,3	0.87	0
3	SO4	I	231	-	4,4,4	0.14	0	6,6,6	0.38	0
4	BCT	G	231	-	2,3,3	0.59	0	2,3,3	0.28	0
4	BCT	C	232	-	2,3,3	0.56	0	2,3,3	0.61	0
3	SO4	E	231	-	4,4,4	0.15	0	6,6,6	0.44	0
3	SO4	K	231	-	4,4,4	0.18	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BCT	H	233	-	2,3,3	0.53	0	2,3,3	0.43	0
4	BCT	E	233	-	2,3,3	0.65	0	2,3,3	0.79	0

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.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	232	BCT	1	0
3	A	231	SO4	1	0
3	B	232	SO4	1	0
4	B	233	BCT	2	0
4	G	231	BCT	1	0
4	C	232	BCT	3	0
4	E	233	BCT	1	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](#)

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	208/229 (90%)	0.58	20 (9%) 8 7	28, 34, 48, 57	0
1	B	212/229 (92%)	0.66	26 (12%) 4 3	27, 33, 46, 51	0
1	C	208/229 (90%)	0.62	21 (10%) 7 6	27, 33, 48, 54	0
1	D	213/229 (93%)	0.64	29 (13%) 3 2	27, 33, 45, 52	0
1	E	212/229 (92%)	0.81	36 (16%) 1 1	27, 32, 44, 48	0
1	F	208/229 (90%)	0.67	26 (12%) 3 3	27, 32, 44, 51	0
1	G	214/229 (93%)	0.90	34 (15%) 1 1	27, 34, 46, 49	0
1	H	209/229 (91%)	0.69	27 (12%) 3 3	28, 34, 46, 60	0
1	I	210/229 (91%)	0.97	35 (16%) 1 1	30, 37, 50, 54	0
1	J	205/229 (89%)	0.65	21 (10%) 6 6	28, 35, 47, 53	0
1	K	209/229 (91%)	1.11	39 (18%) 1 1	32, 38, 49, 55	0
1	L	206/229 (89%)	0.73	29 (14%) 2 2	30, 36, 47, 50	0
All	All	2514/2748 (91%)	0.75	343 (13%) 3 2	27, 34, 47, 60	0

The worst 5 of 343 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	20	GLU	8.6
1	K	135	GLY	7.0
1	J	20	GLU	6.2
1	I	20	GLU	6.1
1	C	219	ASN	6.0

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 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
3	SO4	K	231	5/5	0.61	0.28	89,91,91,91	0
3	SO4	E	232	5/5	0.76	0.26	73,74,75,76	0
3	SO4	L	231	5/5	0.80	0.18	75,77,77,78	0
3	SO4	H	231	5/5	0.81	0.28	71,73,74,75	0
3	SO4	H	232	5/5	0.82	0.21	75,78,78,79	0
3	SO4	I	231	5/5	0.84	0.23	73,74,75,76	0
4	BCT	G	231	4/4	0.89	0.14	40,40,40,40	0
3	SO4	E	231	5/5	0.91	0.16	64,67,68,68	0
4	BCT	C	232	4/4	0.92	0.38	18,19,19,20	4
3	SO4	D	231	5/5	0.93	0.18	67,69,70,70	0
3	SO4	J	231	5/5	0.93	0.14	72,72,74,74	0
3	SO4	A	231	5/5	0.95	0.25	38,38,39,39	5
4	BCT	D	232	4/4	0.95	0.10	41,41,41,42	0
2	ZN	I	230	1/1	0.95	0.04	36,36,36,36	0
4	BCT	K	232	4/4	0.95	0.09	37,38,38,38	0
3	SO4	B	231	5/5	0.96	0.13	57,59,60,60	0
4	BCT	B	233	4/4	0.96	0.13	45,46,46,46	0
4	BCT	L	232	4/4	0.96	0.08	41,41,41,41	0
2	ZN	A	230	1/1	0.97	0.04	31,31,31,31	0
4	BCT	I	232	4/4	0.97	0.10	43,44,44,45	0
4	BCT	J	232	4/4	0.97	0.07	41,41,42,42	0
3	SO4	C	231	5/5	0.97	0.10	60,62,62,62	0
4	BCT	E	233	4/4	0.97	0.08	38,38,38,39	0
4	BCT	H	233	4/4	0.98	0.06	38,38,38,39	0
2	ZN	G	230	1/1	0.98	0.05	31,31,31,31	0
2	ZN	K	230	1/1	0.98	0.05	36,36,36,36	0
4	BCT	F	231	4/4	0.98	0.06	38,38,38,38	0
3	SO4	B	232	5/5	0.98	0.07	55,55,55,56	0
2	ZN	D	230	1/1	0.99	0.03	30,30,30,30	0
2	ZN	J	230	1/1	0.99	0.03	33,33,33,33	0
2	ZN	E	230	1/1	0.99	0.04	28,28,28,28	0
2	ZN	L	230	1/1	0.99	0.03	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	F	230	1/1	0.99	0.03	31,31,31,31	0
2	ZN	B	230	1/1	0.99	0.02	31,31,31,31	0
2	ZN	H	230	1/1	0.99	0.03	32,32,32,32	0
2	ZN	C	230	1/1	1.00	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.