Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 02:37 AM EDT

PDB ID	:	6VJ3
Title	:	Carbonic Anhydrase II in complex with pyrimidine-based inhibitor
Authors	:	Lomelino, C.L.; McKenna, R.
Deposited on	:	2020-01-14
Resolution	:	1.35 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 (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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
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)	:	2.35.1

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 1.35 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

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
3	QYA	A	302[A]	-	X	-	-
3	QYA	A	302[B]	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4394 atoms, of which 2039 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.

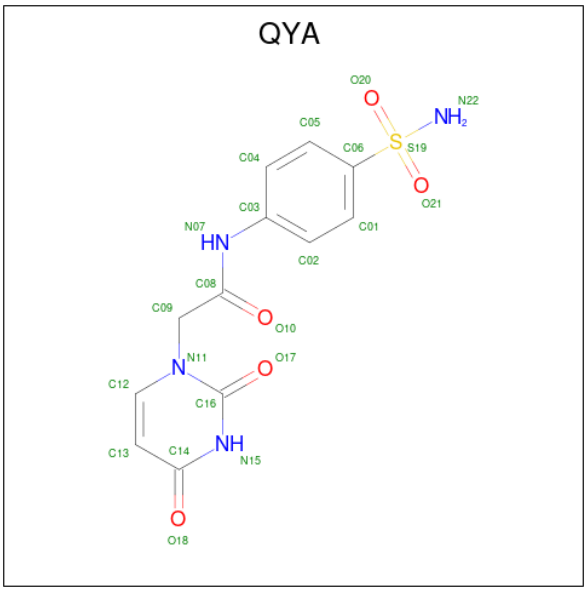
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	258	4068	1321	2009	355	381	2	0	0	0

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

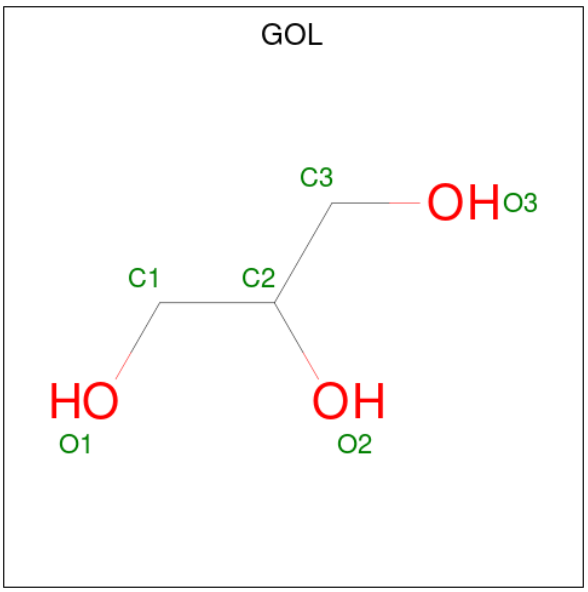
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is 2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-N-(4-sulfamoylphenyl)acetamide (three-letter code: QYA) (formula: $C_{12}H_{12}N_4O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
3	A	1	66	24	22	8	10	2	0	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	14	3	8	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	245	245	245	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.52Å 41.40Å 72.16Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	32.15 – 1.35	Depositor
% Data completeness (in resolution range)	98.5 (32.15-1.35)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.35Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.151 , 0.173	Depositor
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.165	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
Total number of atoms	4394	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
3	QYA	A	302[A]	2	23,23,23	2.46	11 (47%)	33,33,33	2.37	16 (48%)
4	GOL	A	303	-	5,5,5	0.82	0	5,5,5	1.14	1 (20%)
3	QYA	A	302[B]	2	23,23,23	2.45	12 (52%)	33,33,33	2.80	14 (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
3	QYA	A	302[A]	2	-	2/14/14/14	0/2/2/2
4	GOL	A	303	-	-	0/4/4/4	-
3	QYA	A	302[B]	2	-	4/14/14/14	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[A]	QYA	C08-N07	4.94	1.46	1.35
3	A	302[B]	QYA	C08-N07	4.93	1.46	1.35
3	A	302[A]	QYA	S19-N22	4.69	1.69	1.60
3	A	302[B]	QYA	S19-N22	4.57	1.69	1.60
3	A	302[A]	QYA	C14-N15	-4.13	1.31	1.38
3	A	302[B]	QYA	C06-S19	3.96	1.83	1.77
3	A	302[B]	QYA	C14-N15	-3.74	1.31	1.38
3	A	302[A]	QYA	C06-S19	3.67	1.82	1.77
3	A	302[A]	QYA	O18-C14	-3.00	1.18	1.24
3	A	302[A]	QYA	C16-N15	-2.99	1.32	1.38
3	A	302[B]	QYA	O18-C14	-2.88	1.18	1.24
3	A	302[B]	QYA	C03-N07	2.83	1.47	1.41
3	A	302[A]	QYA	C13-C14	-2.77	1.37	1.43
3	A	302[B]	QYA	C13-C14	-2.74	1.37	1.43
3	A	302[B]	QYA	C16-N15	-2.69	1.33	1.38
3	A	302[A]	QYA	C16-N11	-2.67	1.34	1.37
3	A	302[B]	QYA	O10-C08	-2.57	1.18	1.23
3	A	302[B]	QYA	C16-N11	-2.56	1.34	1.37
3	A	302[A]	QYA	C12-N11	-2.48	1.33	1.37
3	A	302[A]	QYA	C03-N07	2.46	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[B]	QYA	O17-C16	-2.21	1.19	1.23
3	A	302[A]	QYA	O17-C16	-2.16	1.19	1.23
3	A	302[B]	QYA	C12-N11	-2.15	1.33	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302[B]	QYA	C08-C09-N11	9.55	123.65	111.22
3	A	302[A]	QYA	N15-C16-N11	5.08	119.51	114.86
3	A	302[A]	QYA	O21-S19-O20	-5.03	110.49	118.76
3	A	302[B]	QYA	N15-C16-N11	4.99	119.42	114.86
3	A	302[B]	QYA	C09-C08-N07	4.74	123.03	114.12
3	A	302[B]	QYA	O21-S19-O20	-4.12	111.99	118.76
3	A	302[A]	QYA	C08-C09-N11	-4.10	105.88	111.22
3	A	302[B]	QYA	C09-N11-C16	3.92	122.43	117.84
3	A	302[B]	QYA	C13-C14-N15	3.41	119.94	114.84
3	A	302[A]	QYA	O20-S19-N22	3.37	112.36	107.36
3	A	302[B]	QYA	C14-N15-C16	-3.31	122.21	126.58
3	A	302[A]	QYA	C14-N15-C16	-3.20	122.36	126.58
3	A	302[A]	QYA	C13-C14-N15	3.19	119.62	114.84
3	A	302[A]	QYA	C09-C08-N07	3.15	120.03	114.12
3	A	302[A]	QYA	C13-C12-N11	-3.12	119.51	122.44
3	A	302[B]	QYA	O18-C14-C13	-3.06	119.78	125.16
3	A	302[A]	QYA	C05-C06-S19	3.00	124.08	119.73
3	A	302[A]	QYA	C03-N07-C08	-2.97	122.30	127.50
3	A	302[A]	QYA	O21-S19-N22	2.86	111.60	107.36
3	A	302[B]	QYA	C03-N07-C08	-2.77	122.64	127.50
3	A	302[A]	QYA	O18-C14-C13	-2.69	120.43	125.16
3	A	302[B]	QYA	O20-S19-N22	2.56	111.15	107.36
3	A	302[A]	QYA	O17-C16-N11	-2.49	120.66	122.85
3	A	302[B]	QYA	O17-C16-N11	-2.44	120.71	122.85
3	A	302[B]	QYA	C13-C12-N11	-2.39	120.20	122.44
3	A	302[A]	QYA	O10-C08-C09	-2.28	117.08	121.08
3	A	302[A]	QYA	O20-S19-C06	-2.28	104.81	107.35
3	A	302[B]	QYA	O10-C08-N07	-2.24	119.55	123.63
4	A	303	GOL	C3-C2-C1	2.17	120.14	111.70
3	A	302[B]	QYA	O10-C08-C09	-2.16	117.30	121.08
3	A	302[A]	QYA	C01-C06-S19	-2.10	116.69	119.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

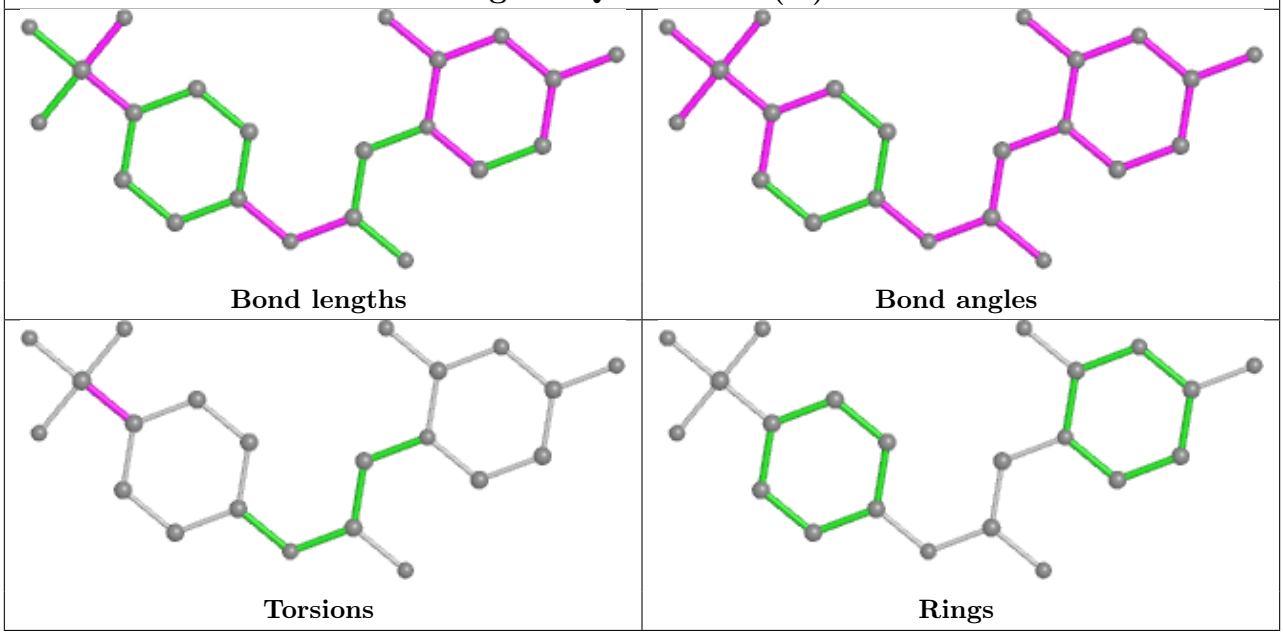
Mol	Chain	Res	Type	Atoms
3	A	302[B]	QYA	N07-C08-C09-N11
3	A	302[B]	QYA	O10-C08-C09-N11
3	A	302[B]	QYA	C05-C06-S19-O21
3	A	302[B]	QYA	C01-C06-S19-O21
3	A	302[A]	QYA	C05-C06-S19-O21
3	A	302[A]	QYA	C01-C06-S19-O21

There are no ring outliers.

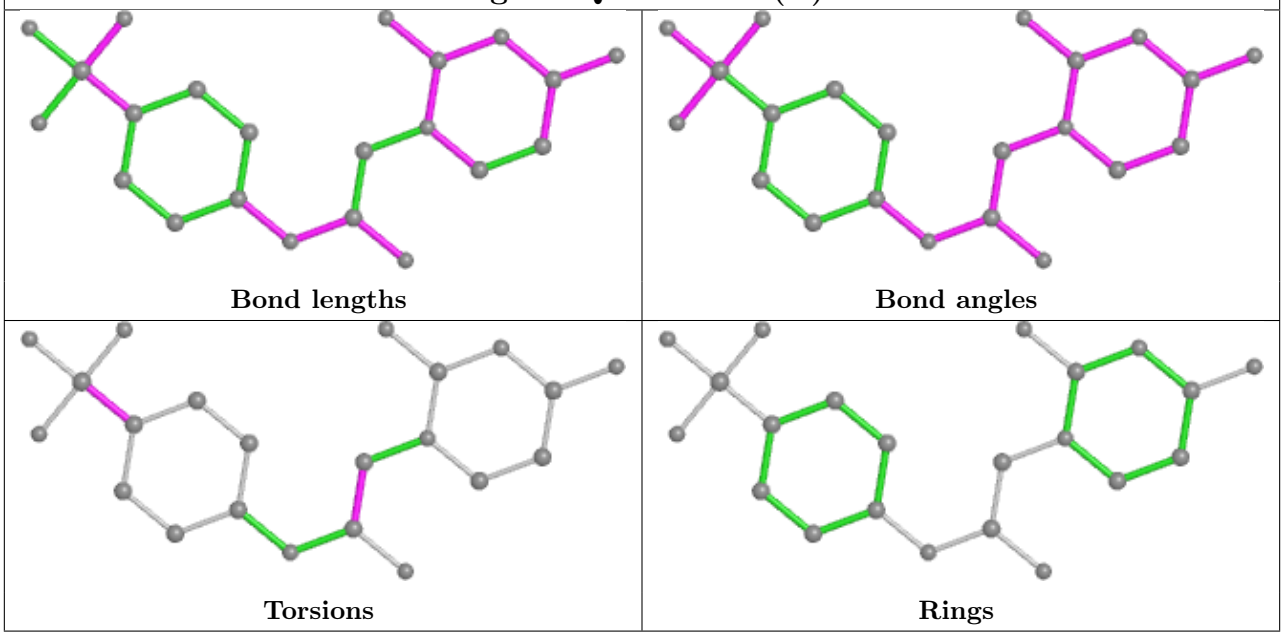
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand QYA A 302 (A)



Ligand QYA A 302 (B)



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.