

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 11:58 PM EDT

PDB ID : 6UGQ

Title: Human Carbonic Anhydrase IX-mimic complexed with SB4-206

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Deposited on : 2019-09-26

Resolution : 1.30 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 as 541be (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 1.30 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:

Mo	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Q7A	A	302	-	X	-	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4298 atoms, of which 2014 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 IX-mimic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	257	Total 4061	C 1315	H 2006	N 353	O 385	S 2	0	3	0

There are 7 discrepancies between the modelled and reference sequences:

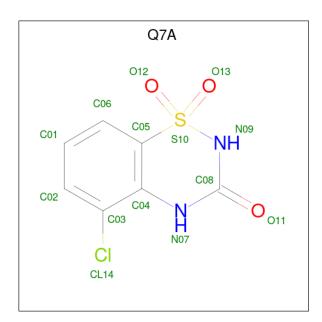
Chain	Residue Modelled		Actual	Comment	Reference	
A	65	SER	ALA	engineered mutation	UNP P00918	
A	67	GLN	ASN	engineered mutation	UNP P00918	
A	69 THR		GLU	engineered mutation	UNP P00918	
A	91	LEU	ILE	engineered mutation	UNP P00918	
A	131 VAL		PHE	engineered mutation	UNP P00918	
A	A 170 GLU		LYS	engineered mutation	UNP P00918	
A	204	ALA	LEU	engineered mutation	UNP P00918	

• 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

• Molecule 3 is 5-chloro-1lambda 6 ,2,4-benzothiadiazine-1,1,3(2H,4H)-trione (three-letter code: Q7A) (formula: C₇H₅ClN₂O₃S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Atoms				ZeroOcc	AltConf		
9	Λ	1	Total	С	Cl	Н	N	О	S	0	0
3	A	1	18	7	1	4	2	3	1		0
9	Λ	1	Total	С	Cl	Н	N	О	S	0	0
3	A	1	18	7	1	4	2	3	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	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	42.13Å 41.45Å 72.03Å	Depositor		
a, b, c, α , β , γ	90.00° 103.95° 90.00°	Depositor		
Resolution (Å)	30.44 - 1.30	Depositor		
% Data completeness	92.6 (30.44-1.30)	Depositor		
(in resolution range)	,	•		
R_{merge}	0.03	Depositor		
R_{sym}	(Not available)	Depositor		
$< I/\sigma(I) > 1$	2.28 (at 1.31Å)	Xtriage		
Refinement program	PHENIX 1.11.1_2575	Depositor		
R, R_{free}	0.153 , 0.163	Depositor		
Wilson B-factor (\mathring{A}^2)	12.1	Xtriage		
Anisotropy	0.092	Xtriage		
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage		
Estimated twinning fraction	No twinning to report.	Xtriage		
Total number of atoms	4298	wwPDB-VP		
Average B, all atoms (\mathring{A}^2)	19.0	wwPDB-VP		

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.97% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	В	ond leng	gths	В	ond ang	gles
			nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	Q7A	A	303	-	15,15,15	5.96	9 (60%)	20,23,23	4.97	7 (35%)
3	Q7A	A	302	2	15,15,15	5.71	11 (73%)	20,23,23	5.84	13 (65%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Q7A	A	303	-	-	-	0/1/2/2
3	Q7A	A	302	2	-	-	0/1/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(\AA)$	Ideal(Å)
3	A	303	Q7A	C05-S10	-16.35	1.61	1.75
3	A	302	Q7A	C05-S10	-14.93	1.62	1.75
3	A	303	Q7A	C08-N07	10.15	1.55	1.36
3	A	302	Q7A	C08-N07	8.59	1.52	1.36
3	A	303	Q7A	C04-N07	8.48	1.57	1.39
3	A	302	Q7A	C04-N07	7.58	1.55	1.39
3	A	302	Q7A	C08-N09	6.93	1.45	1.36
3	A	303	Q7A	C08-N09	6.91	1.45	1.36
3	A	302	Q7A	O12-S10	4.48	1.48	1.43
3	A	303	Q7A	S10-N09	-4.00	1.58	1.62
3	A	302	Q7A	O13-S10	3.92	1.48	1.43
3	A	302	Q7A	O11-C08	-3.86	1.15	1.23
3	A	302	Q7A	S10-N09	-3.79	1.58	1.62
3	A	302	Q7A	C03-CL14	3.21	1.81	1.73
3	A	303	Q7A	O13-S10	2.93	1.46	1.43
3	A	303	Q7A	O12-S10	2.38	1.46	1.43
3	A	303	Q7A	O11-C08	-2.31	1.18	1.23
3	A	302	Q7A	C01-C06	-2.11	1.34	1.38
3	A	302	Q7A	C01-C02	2.09	1.43	1.38
3	A	303	Q7A	C03-CL14	2.03	1.78	1.73

All (20) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	303	Q7A	C05-S10-N09	15.81	115.60	102.13
3	A	302	Q7A	C05-S10-N09	13.42	113.56	102.13
3	A	302	Q7A	O12-S10-N09	-13.18	97.51	108.26
3	A	302	Q7A	C03-C04-N07	-9.34	116.19	121.88
3	A	303	Q7A	O12-S10-N09	-9.24	100.72	108.26
3	A	303	Q7A	C03-C04-N07	-9.17	116.30	121.88
3	A	302	Q7A	O13-S10-N09	8.52	115.20	108.26
3	A	302	Q7A	C04-C05-S10	5.25	123.09	119.04
3	A	302	Q7A	C03-C04-C05	4.76	123.61	116.18
3	A	302	Q7A	C02-C03-C04	-4.66	114.54	121.96
3	A	302	Q7A	O13-S10-O12	-4.53	113.84	118.46
3	A	302	Q7A	N09-C08-N07	4.52	123.04	115.79
3	A	302	Q7A	O11-C08-N07	-4.50	115.59	122.08
3	A	303	Q7A	C04-C05-S10	4.40	122.44	119.04
3	A	302	Q7A	C02-C03-CL14	4.12	126.67	118.41
3	A	303	Q7A	C03-C04-C05	3.88	122.24	116.18
3	A	303	Q7A	O13-S10-O12	-3.37	115.02	118.46
3	A	302	Q7A	O12-S10-C05	-3.29	105.22	109.29
3	A	303	Q7A	N09-C08-N07	3.16	120.85	115.79
3	A	302	Q7A	C06-C05-S10	-2.33	115.73	119.37

There are no chirality outliers.

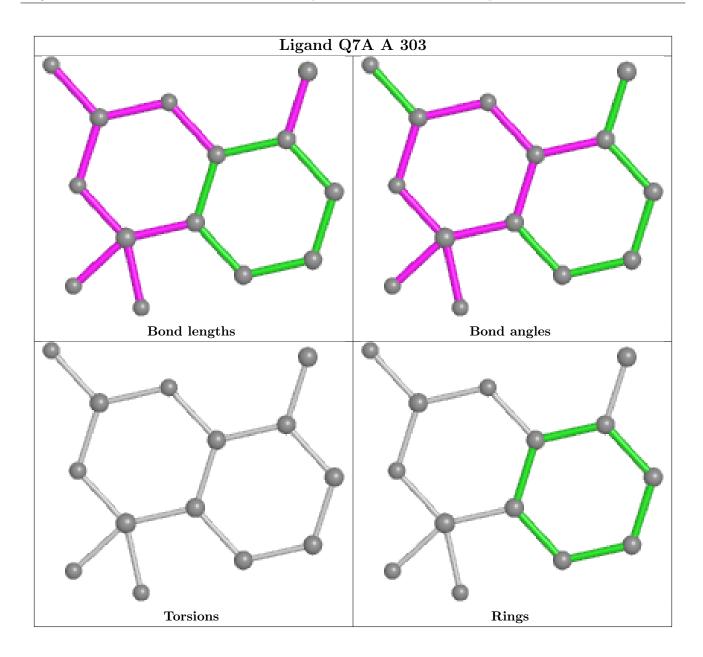
There are no torsion outliers.

There are no ring outliers.

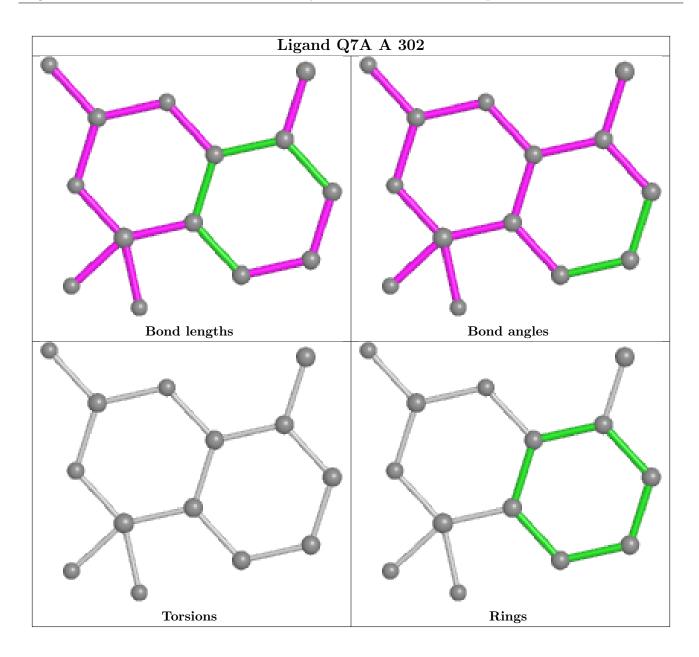
No monomer is involved in short contacts.

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.









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.

