

wwPDB X-ray Structure Validation Summary Report (i)

Sep 4, 2024 – 01:15 pm BST

PDB ID : 8QF7

Title: Human Carbonic Anhydrase II in complex with (3-((N-(4-sulfamoylbenzyl)ph

enylsulfonamido)methyl)phenyl)glycine

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Deposited on : 2023-09-04

Resolution : 1.23 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 3.0

buster-report : 1.1.7 (2018)

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.002 (Gargrove)

Density-Fitness : 1.0.11

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

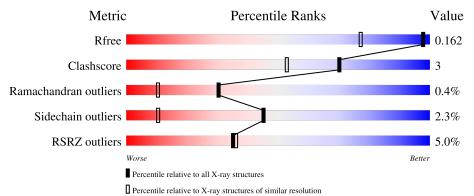
Validation Pipeline (wwPDB-VP) : 2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.23 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	164625	1745 (1.24-1.20)
Clashscore	180529	1895 (1.24-1.20)
Ramachandran outliers	177936	1845 (1.24-1.20)
Sidechain outliers	177891	1844 (1.24-1.20)
RSRZ outliers	164620	1744 (1.24-1.20)

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 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% 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					
			5%					
1	AAA	260	88%	10%	••			



2 Entry composition (i)

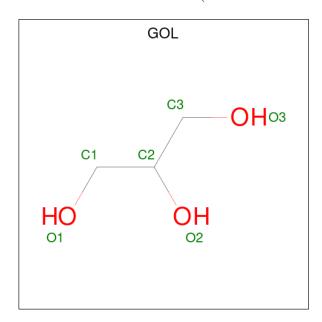
There are 6 unique types of molecules in this entry. The entry contains 2429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	AAA	258	Total 2127	C 1372	N 361	O 392	S 2	0	18	0

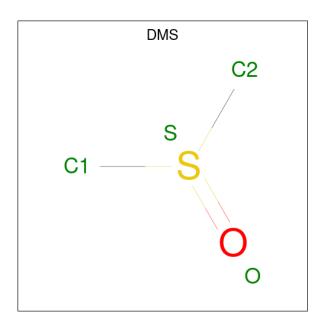
• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total 6	C 3	O 3	0	0

• Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



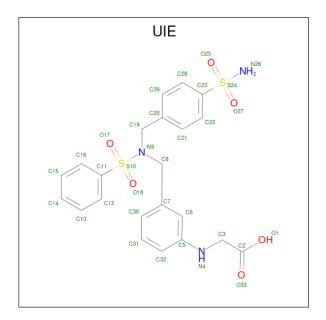


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total 4	C 2	O 1	S 1	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Zn 1 1	0	0

• Molecule 5 is 2-[[3-[[phenylsulfonyl-[(4-sulfamoylphenyl)methyl]amino]methyl]phenyl]amino]ethanoic acid (three-letter code: UIE) (formula: $C_{22}H_{23}N_3O_6S_2$) (labeled as "Ligand of Interest" by depositor).





\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	
E	ΛΛΛ	1	Total	С	N	О	S	E	0
5	AAA	1	33	22	3	6	2	9	

• Molecule 6 is water.

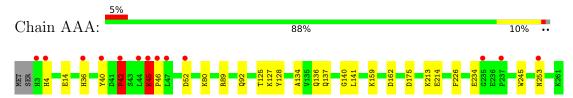
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	258	Total O 258 258	0	0



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





4 Data and refinement statistics (i)

Property	Value	Source			
Space group	P 1 21 1	Depositor			
Cell constants	42.44Å 41.46Å 72.41Å	Donositor			
a, b, c, α , β , γ	90.00° 104.41° 90.00°	Depositor			
Resolution (Å)	40.11 - 1.23	Depositor			
resolution (A)	40.11 - 1.23	Depositor Depositor EDS Depositor EDS Depositor Depositor Depositor Xtriage Depositor Depositor Depositor Variage Depositor Decc wwPDB-VP Xtriage Xtriage EDS Xtriage			
% Data completeness	84.6 (40.11-1.23)	Depositor			
(in resolution range)	84.6 (40.11-1.23)	EDS			
R_{merge}	0.04	Depositor			
R_{sym}	(Not available)	Depositor			
$< I/\sigma(I) > 1$	2.17 (at 1.22Å)	Xtriage			
Refinement program	REFMAC 5.8.0258	Depositor			
R, R_{free}	0.117 , 0.152	Depositor			
it, it _{free}	0.128 , 0.162	DCC			
R_{free} test set	3606 reflections (4.98%)	wwPDB-VP			
Wilson B-factor (Å ²)	10.7				
Anisotropy	0.705	Xtriage			
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 48.9	EDS			
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage			
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage			
F_o, F_c correlation	0.98	EDS			
Total number of atoms	2429	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 8.86% 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.

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: UIE, GOL, DMS, 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	Bo	nd lengths	Bo	nd angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	AAA	1.03	13/2231 (0.6%)	1.10	8/3021 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	Ideal(A)
1	AAA	52	ASP	CG-OD2	16.25	1.62	1.25
1	AAA	14	GLU	CD-OE2	14.03	1.41	1.25
1	AAA	214	GLU	CD-OE1	-6.88	1.18	1.25
1	AAA	46	PRO	C-O	-6.30	1.10	1.23
1	AAA	45	LYS	C-N	6.17	1.46	1.34

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
1	AAA	52	ASP	CB-CG-OD2	-17.15	102.86	118.30
1	AAA	52	ASP	CB-CG-OD1	14.54	131.39	118.30
1	AAA	226	PHE	CB-CG-CD1	9.23	127.26	120.80
1	AAA	141	LEU	CB-CG-CD2	6.19	121.52	111.00
1	AAA	226	PHE	CB-CG-CD2	-5.43	117.00	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	AAA	42	PRO	Mainchain

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	AAA	2127	0	2115	11	0
2	AAA	6	0	8	2	0
3	AAA	4	0	6	2	0
4	AAA	1	0	0	0	0
5	AAA	33	0	0	0	0
6	AAA	258	0	0	9	0
All	All	2429	0	2129	14	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 3.

The worst 5 of 14 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:AAA:213[A]:LYS:HE3	6:AAA:501:HOH:O	1.35	1.23
1:AAA:89[A]:ARG:HG3	6:AAA:572:HOH:O	1.67	0.92
2:AAA:301:GOL:H31	6:AAA:419:HOH:O	1.88	0.73
1:AAA:89[A]:ARG:CG	6:AAA:572:HOH:O	2.32	0.69
1:AAA:40:TYR:CZ	1:AAA:42:PRO:HA	2.30	0.65

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	AAA	270/260 (104%)	262 (97%)	7 (3%)	1 (0%)	30 10	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	45	LYS

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	Percer	Percentiles	
1	AAA	235/225 (104%)	230 (98%)	5 (2%)	48	12	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	4	HIS
1	AAA	45	LYS
1	AAA	80	LYS
1	AAA	92	GLN
1	AAA	159	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 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).

Mal	Mol Type		Res	Link	Bo	ond leng	$ ag{ths}$	Ths Bond angles		
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	AAA	301	-	5,5,5	0.21	0	5,5,5	0.51	0
3	DMS	AAA	302	-	3,3,3	1.70	1 (33%)	3,3,3	2.36	1 (33%)
5	UIE	AAA	304	4	35,35,35	1.49	2 (5%)	50,50,50	1.43	9 (18%)

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
2	GOL	AAA	301	-	-	2/4/4/4	-
5	UIE	AAA	304	4	-	11/31/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
5	AAA	304	UIE	S10-N9	7.19	1.73	1.63
5	AAA	304	UIE	C5-N4	-2.70	1.30	1.38
3	AAA	302	DMS	O-S	2.42	1.66	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	AAA	304	UIE	C7-C8-N9	4.52	121.23	112.15
3	AAA	302	DMS	O-S-C1	3.95	126.69	106.54

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
5	AAA	304	UIE	C8-N9-S10	3.43	125.38	117.35
5	AAA	304	UIE	C32-C5-N4	-2.56	115.67	120.97
5	AAA	304	UIE	O25-S24-N26	2.47	111.03	107.36

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	304	UIE	C2-C3-N4-C5
2	AAA	301	GOL	C1-C2-C3-O3
5	AAA	304	UIE	C22-C23-S24-O27
5	AAA	304	UIE	C22-C23-S24-N26
5	AAA	304	UIE	C28-C23-S24-O27

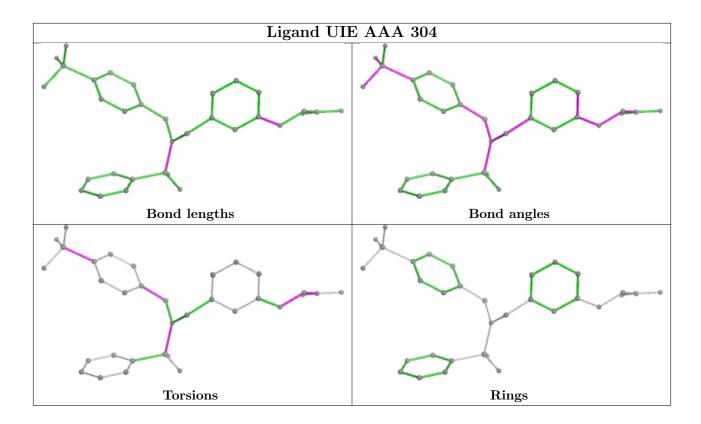
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	301	GOL	2	0
3	AAA	302	DMS	2	0

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.





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, 95^{th} 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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	AAA	258/260 (99%)	-0.25	13 (5%) 35 3	7, 13, 39, 135	15 (5%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	46	PRO	9.8
1	AAA	40	TYR	5.9
1	AAA	3	HIS	5.1
1	AAA	42	PRO	4.0
1	AAA	45	LYS	3.7

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	GOL	AAA	301	6/6	0.75	0.15	43,49,57,61	0
3	DMS	AAA	302	4/4	0.88	0.14	19,20,45,54	0

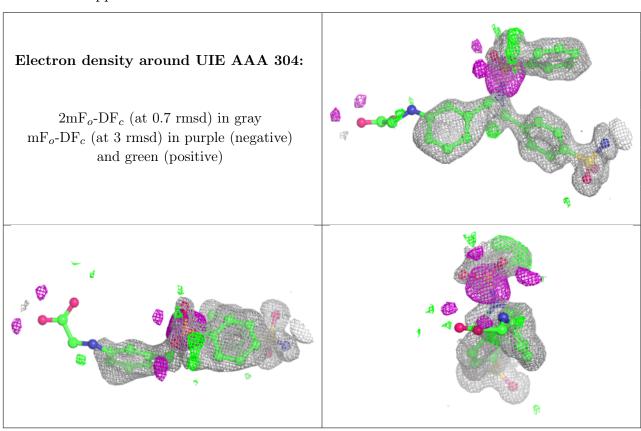
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	UIE	AAA	304	33/33	0.97	0.10	7,31,100,132	5
4	ZN	AAA	303	1/1	1.00	0.01	7,7,7,7	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

