

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 7, 2023 – 02:14 am GMT

PDB ID	:	8PBU
Title	:	Mutant K1482M of the dihydroorotase domain of human CAD protein bound
		to the inhibitor fluoorotate
Authors	:	del Cano-Ochoa, F.; Ramon-Maiques, S.
Deposited on	:	2023-06-09
Resolution	:	1.67  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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
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)	:	2.36

## PERCENTILES INFOmissingINFO



#### 8PBU

# 1 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5955 atoms, of which 2833 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 CAD protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	362	Total 5632	C 1804	Н 2815	N 491	O 506	S 16	0	20	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1482	MET	LYS	engineered mutation	UNP P27708

• Molecule 2 is 5-FLUORO-2,6-DIOXO-1,2,3,6-TETRAHYDROPYRIMIDINE-4-CARBOXY LIC ACID (three-letter code: FOT) (formula: C<sub>5</sub>H<sub>3</sub>FN<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
2	А	1	Total 14	$\begin{array}{c} \mathrm{C} \\ 5 \end{array}$	F 1	Н 2	N 2	0 4	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	5	Total Zn 5 5	0	0

• Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
4	٨	1	Total	С	Η	0	0	0	
4	-	1	5	1	2	2	0	0	
4	Λ	1	Total	С	Η	0	0	0	
4	Л	1	5	1	2	2	0	0	
4	Λ	1	Total	С	Η	0	0	0	
4	Л	1	5	1	2	2	0	0	
4	Λ	1	Total	С	Η	0	0	0	
4	Л	T	5	1	2	2	0	0	
4	Δ	1	Total	С	Η	0	0	0	
4	Π	1	5	1	2	2	0		
4	Λ	1	Total	С	Η	0	0	0	
4	Л	1	5	1	2	2	0	0	
4	Λ	1	Total	С	Η	0	0	0	
4	Л	1	5	1	2	2	0	0	
4	Δ	1	Total	С	Η	0	0	0	
4	Л	1	5	1	2	2	0	0	

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	264	Total O 264 264	0	0



## SEQUENCE-PLOTS INFOmissingINFO



# 2 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	82.17Å 158.97Å 61.48Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$Posclution(\hat{\lambda})$	48.63 - 1.67	Depositor
Resolution (A)	48.63 - 1.67	EDS
% Data completeness	91.6 (48.63-1.67)	Depositor
(in resolution range)	91.6 (48.63 - 1.67)	EDS
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.85 (at 1.67 Å)	Xtriage
Refinement program	REFMAC v8.0, PHENIX 1.20.1_4487	Depositor
B.B.	0.141 , $0.191$	Depositor
II, II, <i>free</i>	0.152 , $0.197$	DCC
$R_{free}$ test set	2186 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	23.2	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.41 , $43.1$	EDS
L-test for twinning <sup>2</sup>	$ L  > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	5955	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 3 Model quality (i)

## 3.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, KCX, FOT, FMT

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.30	0/2929	0.55	0/4001	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 3.2 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	А	2817	2815	2793	14	0
2	А	12	2	2	0	0
3	А	5	0	0	0	0
4	А	24	16	8	0	0
5	А	264	0	0	0	0
All	All	3122	2833	2803	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 2.

All (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:A:1593:GLN:O	1:A:1596[B]:VAL:HG12	1.89	0.73
1:A:1596[B]:VAL:HG13	1:A:1623:LEU:HD23	1.74	0.69
1:A:1588[A]:VAL:CG1	1:A:1613:CYS:SG	2.89	0.61
1:A:1588[B]:VAL:HG22	1:A:1613:CYS:SG	2.43	0.58
1:A:1596[B]:VAL:HG13	1:A:1623:LEU:CD2	2.34	0.55
1:A:1798:GLN:HG2	1:A:1800:LEU:HD21	1.91	0.53
1:A:1556:KCX:CD	1:A:1588[B]:VAL:HG13	2.43	0.48
1:A:1474:LEU:HD22	1:A:1488:GLY:HA3	1.97	0.47
1:A:1556:KCX:HD3	1:A:1588[B]:VAL:HG13	1.99	0.44
1:A:1640:PRO:HG2	1:A:1710:MET:HB2	2.01	0.43
1:A:1472[B]:VAL:HG13	1:A:1687:HIS:HB3	2.01	0.42
1:A:1758:TRP:CZ3	1:A:1760[B]:ILE:HD13	2.55	0.41
1:A:1472[B]:VAL:HG11	1:A:1474:LEU:HD21	2.01	0.41
1:A:1711:LEU:HB3	1:A:1712:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

### 3.3 Torsion angles (i)

#### 3.3.1 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	А	376/362~(104%)	365~(97%)	9(2%)	2 (0%)	29 12	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1614	HIS
1	А	1706	GLY

#### 3.3.2 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	А	301/296~(102%)	298~(99%)	3 (1%)	76 65	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1569	ASP
1	А	1614	HIS
1	А	1814	GLN

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

#### 3.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	5 Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
1	KCX	А	1556	1,3	9,11,12	0.85	0	5,12,14	1.65	1 (20%)

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
1	KCX	А	1556	1,3	-	0/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1556	KCX	OQ1-CX-NZ	-3.66	119.28	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	1556	KCX	2	0

## 3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 3.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	Turne	Chain	Dec	Link	Bo	ond leng	ths	В	ond ang	les
INIOI	Type	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FMT	А	1914	3	$2,\!2,\!2$	0.72	0	$1,\!1,\!1$	0.47	0
4	FMT	А	1910	-	2,2,2	0.75	0	$1,\!1,\!1$	0.45	0
4	FMT	А	1909	-	2,2,2	0.73	0	$1,\!1,\!1$	0.44	0
4	FMT	А	1911	-	2,2,2	0.73	0	$1,\!1,\!1$	0.47	0
4	FMT	A	1912	3	$2,\!2,\!2$	0.72	0	$1,\!1,\!1$	0.46	0
2	FOT	А	1901	-	11,12,12	3.55	8 (72%)	$11,\!17,\!17$	<mark>3.23</mark>	5 (45%)
4	FMT	A	1913	-	2,2,2	0.77	0	1,1,1	0.49	0



Mol /	Turne	Chain	Dec	Tiple	Bond lengths			В	ond ang	les
IVIOI	туре	Chain	nes	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FMT	A	1908	3	2,2,2	0.72	0	$1,\!1,\!1$	0.47	0
4	FMT	А	1907	-	2,2,2	0.71	0	1,1,1	0.45	0

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	FOT	А	1901	-	-	0/4/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	1901	FOT	C2-N1	6.40	1.48	1.37
2	А	1901	FOT	C2-N3	6.11	1.48	1.37
2	А	1901	FOT	C6-C5	3.97	1.49	1.44
2	А	1901	FOT	C6-N1	3.60	1.45	1.38
2	А	1901	FOT	C4-N3	3.22	1.45	1.38
2	А	1901	FOT	C4-C41	2.83	1.52	1.48
2	А	1901	FOT	O6-C6	-2.26	1.19	1.23
2	А	1901	FOT	O2-C2	-2.00	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1901	FOT	C5-C6-N1	6.88	119.79	112.60
2	А	1901	FOT	O6-C6-C5	-5.77	119.92	125.63
2	А	1901	FOT	C6-N1-C2	-3.87	120.77	126.34
2	А	1901	FOT	O41-C41-C4	2.85	121.46	116.76
2	А	1901	FOT	N1-C2-N3	2.27	119.45	115.80

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.



#### 3.7 Other polymers (i)

There are no such residues in this entry.



## 3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 4 Fit of model and data (i)

## 4.1 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	<RSRZ $>$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	361/362~(99%)	-0.12	9 (2%) 57	60	18, 26, 42, 54	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	А	1698[B]	SER	3.5	
1	А	1563	PHE	3.2	
1	А	1696[A]	CYS	2.8	
1	А	1479	GLY	2.4	
1	А	1651	GLU	2.4	
1	А	1648	ASP	2.4	
1	А	1564	SER	2.3	
1	А	1661	ARG	2.1	
1	А	1650	LEU	2.1	

## 4.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
1	KCX	А	1556	12/13	0.96	0.07	17,25,32,32	0

## 4.3 Carbohydrates (i)

There are no monosaccharides in this entry.



## 4.4 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	FMT	A	1907	3/3	0.93	0.16	56, 56, 67, 69	0
4	FMT	А	1912	3/3	0.93	0.17	36,41,43,50	0
4	FMT	А	1914	3/3	0.93	0.23	43,43,52,54	0
4	FMT	A	1909	3/3	0.94	0.15	51,54,65,65	0
3	ZN	A	1906	1/1	0.95	0.24	$98,\!98,\!98,\!98$	0
2	FOT	А	1901	12/12	0.96	0.09	26,28,34,34	0
4	FMT	А	1913	3/3	0.96	0.14	38,40,46,48	0
4	FMT	А	1910	3/3	0.96	0.10	28,31,34,38	0
4	FMT	А	1908	3/3	0.97	0.09	46,49,59,60	0
4	FMT	А	1911	3/3	0.99	0.10	17,18,21,22	5
3	ZN	А	1903	1/1	1.00	0.06	$25,\!25,\!25,\!25$	0
3	ZN	А	1904	1/1	1.00	0.10	26,26,26,26	1
3	ZN	A	1905	1/1	1.00	0.09	28,28,28,28	0
3	ZN	A	1902	1/1	1.00	0.09	23,23,23,23	0

### 4.5 Other polymers (i)

There are no such residues in this entry.

