

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

Feb 12, 2024 – 09:53 AM EST

PDB ID : 3ITM

Title: Catalytic domain of hPDE2A

Authors : Pandit, J. Deposited on : 2009-08-28

Resolution : 2.49 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:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$ 

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

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

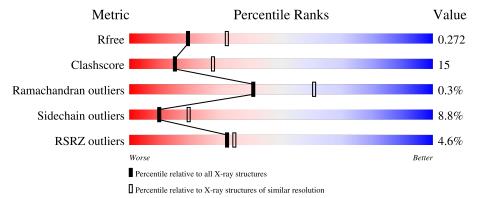
Validation Pipeline (wwPDB-VP) : 2.36

## 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 2.49 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \ resolution} \\ (\#{\rm Entries, \ resolution \ range(\AA)}) \end{array}$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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		
1	A	345	63%	20%	• • 11%
1	В	345	64%	22%	6% 8%
1	С	345	<del>7%</del> 63%	20%	6% • 10%
1	D	345	61%	26%	5% • 8%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10447 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 cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Λ	307	Total	С	N	О	S	0	0	0	
1	A	307	2514	1605	429	455	25	0	0	U	
1	В	318	Total	С	N	О	S	0	0	0	
1	Ъ	310	2609	1662	446	476	25		0	0	
1	С	310	Total	С	N	О	S	0	0	0	
1		310	2548	1626	432	465	25	0	0		
1	D	210	Total	С	N	О	S	0	0	0	
1	$1 \mid D$	318	2609	1662	446	476	25				

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	GLY	-	expression tag	UNP O00408
A	576	SER	-	expression tag	UNP O00408
A	577	ALA	-	expression tag	UNP O00408
A	578	MET	-	expression tag	UNP O00408
В	575	GLY	-	expression tag	UNP O00408
В	576	SER	-	expression tag	UNP O00408
В	577	ALA	-	expression tag	UNP O00408
В	578	MET	-	expression tag	UNP O00408
С	575	GLY	-	expression tag	UNP O00408
С	576	SER	-	expression tag	UNP O00408
С	577	ALA	-	expression tag	UNP O00408
С	578	MET	-	expression tag	UNP O00408
D	575	GLY	-	expression tag	UNP O00408
D	576	SER		expression tag	UNP O00408
D	577	ALA	-	expression tag	UNP O00408
D	578	MET	-	expression tag	UNP O00408

• 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	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

#### • Molecule 3 is water.

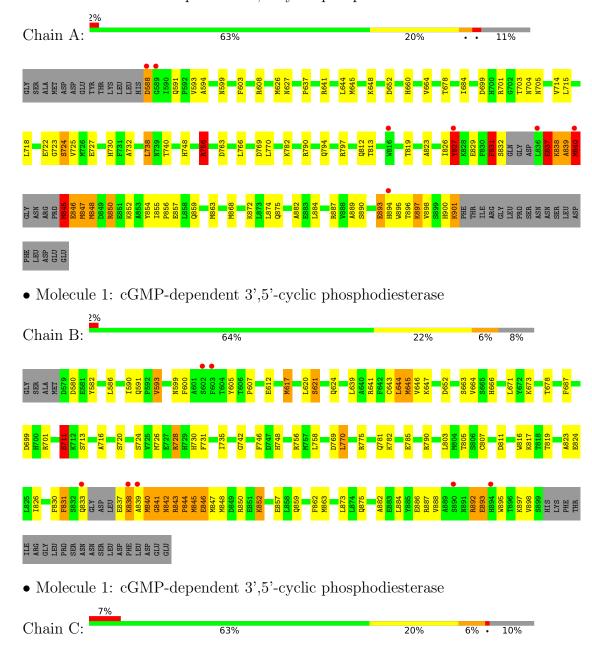
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	43	Total O 43 43	0	0
3	В	65	Total O 65 65	0	0
3	С	25	Total O 25 25	0	0
3	D	30	Total O 30 30	0	0



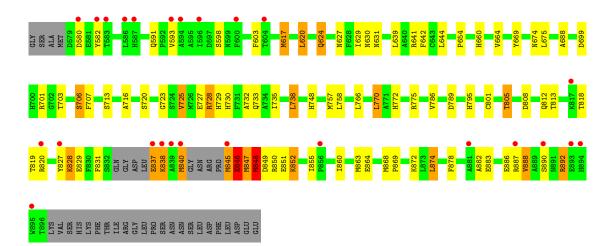
## 3 Residue-property plots (i)

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.

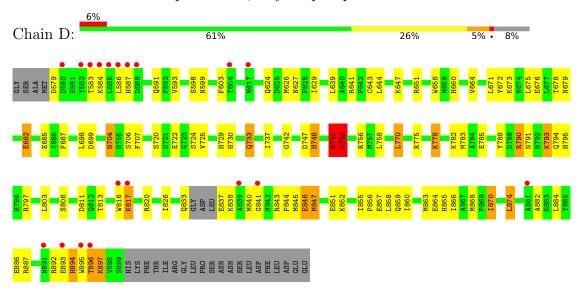
• Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase







 $\bullet$  Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	108.02Å 108.02Å 515.56Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 - 2.49	Depositor
Resolution (A)	49.81 - 2.49	EDS
% Data completeness	84.5 (50.00-2.49)	Depositor
(in resolution range)	84.6 (49.81-2.49)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$< I/\sigma(I) > 1$	2.72 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.227 , 0.286	Depositor
$R, R_{free}$	0.216 , $0.272$	DCC
$R_{free}$ test set	2756 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32, 49.2	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities 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: 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	ond lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	1.81	30/2573~(1.2%)	1.11	17/3468 (0.5%)	
1	В	1.53	$26/2671 \ (1.0\%)$	1.11	17/3602 (0.5%)	
1	С	1.44	24/2608~(0.9%)	1.01	15/3516 (0.4%)	
1	D	1.08	13/2671~(0.5%)	0.96	11/3602 (0.3%)	
All	All	1.48	93/10523~(0.9%)	1.05	60/14188 (0.4%)	

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers	
1	A	0	2	

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
1	A	837	GLU	CD-OE2	40.94	1.70	1.25
1	A	831	PHE	CE1-CZ	29.81	1.94	1.37
1	A	831	PHE	CG-CD2	21.82	1.71	1.38
1	В	831	PHE	CG-CD2	21.14	1.70	1.38
1	С	838	LYS	CE-NZ	21.13	2.01	1.49

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	D	751	ARG	NE-CZ-NH2	17.12	128.86	120.30
1	A	831	PHE	CB-CG-CD1	-14.62	110.56	120.80
1	С	849	ASP	CB-CG-OD1	-12.72	106.86	118.30
1	A	840	MET	CG-SD-CE	-12.61	80.03	100.20

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	843	ARG	NE-CZ-NH2	-11.80	114.40	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	831	PHE	Sidechain
1	A	837	GLU	Sidechain

#### 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	A	2514	0	2462	73	0
1	В	2609	0	2552	87	0
1	С	2548	0	2487	87	0
1	D	2609	0	2552	78	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	A	43	0	0	6	0
3	В	65	0	0	9	0
3	С	25	0	0	3	0
3	D	30	0	0	6	0
All	All	10447	0	10053	307	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 15.

The worst 5 of 307 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:A:901:LYS:CB	1:A:901:LYS:CA	1.75	1.62
1:D:817:LYS:CE	1:D:817:LYS:NZ	1.68	1.57

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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\begin{subarray}{c} \begin{subarray}{c} \begi$
1:A:831:PHE:CZ	1:A:831:PHE:CE1	1.94	1.56
1:A:837:GLU:CB	1:A:837:GLU:CG	1.79	1.55
1:A:838:LYS:CE	1:A:838:LYS:CD	1.81	1.54

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	Perce	ntiles
1	A	301/345 (87%)	285 (95%)	14 (5%)	2 (1%)	22	39
1	В	314/345 (91%)	305 (97%)	8 (2%)	1 (0%)	41	61
1	C	304/345 (88%)	292 (96%)	11 (4%)	1 (0%)	41	61
1	D	314/345 (91%)	301 (96%)	13 (4%)	0	100	100
All	All	1233/1380 (89%)	1183 (96%)	46 (4%)	4 (0%)	41	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	837	GLU
1	A	839	ALA
1	В	711	SER
1	С	580	ASP

#### 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	Perc	centiles
1	A	276/310 (89%)	253 (92%)	23 (8%)	11	22
1	В	287/310 (93%)	265 (92%)	22 (8%)	13	25
1	$\mathbf{C}$	280/310 (90%)	258 (92%)	22 (8%)	12	24
1	D	287/310 (93%)	254 (88%)	33 (12%)	5	11
All	All	1130/1240 (91%)	1030 (91%)	100 (9%)	10	19

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	820	ARG
1	D	598	SER
1	D	896	THR
1	С	846	GLU
1	С	890	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	656	HIS
1	С	795	HIS
1	D	755	GLN
1	С	733	GLN
1	С	875	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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	<rsrz></rsrz>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	307/345 (88%)	0.31	7 (2%) 60 63	37, 42, 48, 56	0
1	В	318/345 (92%)	0.23	7 (2%) 62 65	36, 43, 49, 71	0
1	С	310/345 (89%)	0.45	25 (8%) 12 12	38, 43, 47, 71	0
1	D	318/345 (92%)	0.48	19 (5%) 21 22	37, 42, 49, 74	0
All	All	1253/1380 (90%)	0.37	58 (4%) 32 34	36, 43, 49, 74	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	839	ALA	7.6
1	С	586	LEU	5.1
1	D	586	LEU	5.0
1	С	827	TYR	4.9
1	A	588	ASP	4.9

#### 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	ZN	В	2	1/1	0.99	0.02	30,30,30,30	0
2	ZN	С	3	1/1	0.99	0.03	42,42,42,42	0
2	ZN	D	4	1/1	0.99	0.02	38,38,38,38	0
2	ZN	A	1	1/1	1.00	0.01	33,33,33,33	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

