

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

### Aug 19, 2023 – 11:46 PM EDT

PDB ID : 2G07

Title: X-ray structure of mouse pyrimidine 5'-nucleotidase type 1, phospho-enzyme

intermediate analog with Beryllium fluoride

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Deposited on : 2006-02-11

Resolution : 2.30 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

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

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

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

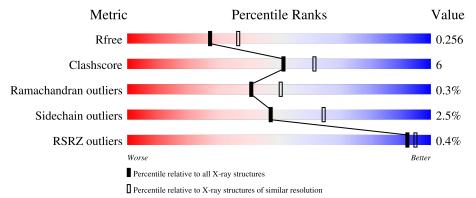
Validation Pipeline (wwPDB-VP) : 2.35

## 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 2.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	297	82%	14%	
1	В	297	86%	11%	



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5200 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 Cytosolic 5'-nucleotidase III.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace			
1	Λ	291	Total	Ве	С	F	N	О	S	Se	0	1	0
1	A	291	2330	1	1487	3	387	439	5	8	U	1	U
1	D	291	Total	Ве	С	F	N	О	S	Se	0	1	0
1	Б	291	2330	1	1487	3	387	439	5	8	0	1	U

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP Q9D020
A	12	MSE	MET	modified residue	UNP Q9D020
A	13	MSE	MET	modified residue	UNP Q9D020
A	49	BFD	ASP	modified residue	UNP Q9D020
A	52	MSE	MET	modified residue	UNP Q9D020
A	110	MSE	MET	modified residue	UNP Q9D020
A	141	MSE	MET	modified residue	UNP Q9D020
A	192	MSE	MET	modified residue	UNP Q9D020
A	245	MSE	MET	modified residue	UNP Q9D020
A	273	MSE	MET	modified residue	UNP Q9D020
В	1	SER	-	cloning artifact	UNP Q9D020
В	12	MSE	MET	modified residue	UNP Q9D020
В	13	MSE	MET	modified residue	UNP Q9D020
В	49	BFD	ASP	modified residue	UNP Q9D020
В	52	MSE	MET	modified residue	UNP Q9D020
В	110	MSE	MET	modified residue	UNP Q9D020
В	141	MSE	MET	modified residue	UNP Q9D020
В	192	MSE	MET	modified residue	UNP Q9D020
В	245	MSE	MET	modified residue	UNP Q9D020
В	273	MSE	MET	modified residue	UNP Q9D020

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	В	1	Total Mg 1 1	0	0

## $\bullet\,$ Molecule 3 is water.

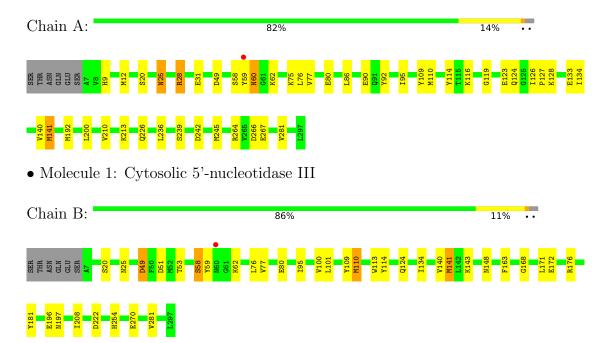
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	274	Total O 274 274	0	0
3	В	264	Total O 264 264	0	0



# 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: Cytosolic 5'-nucleotidase III





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants	134.83Å 134.83Å 38.95Å	D
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	67.42 - 2.30	Depositor
Resolution (A)	44.13 - 2.30	EDS
% Data completeness	93.9 (67.42-2.30)	Depositor
(in resolution range)	93.9 (44.13-2.30)	EDS
$R_{merge}$	0.13	Depositor
$R_{sum}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.91 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D	0.180 , 0.259	Depositor
$R, R_{free}$	0.178 , $0.256$	DCC
$R_{free}$ test set	1673 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , 33.0	EDS
L-test for twinning <sup>2</sup>	$< L >=0.51, < L^2>=0.34$	Xtriage
	0.467 for -h,-k,l	
Estimated twinning fraction	0.024  for h,-h-k,-l	Xtriage
	0.025  for -k,-h,-l	
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.60% 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: BFD, MG

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		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.85	2/2349~(0.1%)	0.77	0/3147	
1	В	0.91	3/2349 (0.1%)	0.80	1/3147 (0.0%)	
All	All	0.88	5/4698 (0.1%)	0.79	1/6294 (0.0%)	

#### All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(Å)
1	В	80	GLU	CD-OE2	13.42	1.40	1.25
1	В	80	GLU	CD-OE1	13.29	1.40	1.25
1	A	80	GLU	CD-OE1	7.87	1.34	1.25
1	В	196	GLU	CD-OE2	6.28	1.32	1.25
1	A	80	GLU	CD-OE2	5.08	1.31	1.25

#### All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	176	ARG	NE-CZ-NH1	5.36	122.98	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2330	0	2343	29	0
1	В	2330	0	2345	23	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	274	0	0	5	0
3	В	264	0	0	3	0
All	All	5200	0	4688	52	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 6.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	$\text{overlap } (\mathring{\mathbf{A}})$
1:B:110:MSE:HE1	1:B:113:TRP:HE3	1.13	1.12
1:B:110:MSE:HE1	1:B:113:TRP:CE3	1.89	1.06
1:A:128:LYS:HE2	3:A:634:HOH:O	1.55	1.04
1:A:110:MSE:HE3	1:A:114:TYR:HE1	1.54	0.73
1:A:110:MSE:CE	1:A:114:TYR:HE1	2.01	0.73
1:B:58:SER:HB2	1:B:62:LYS:O	1.90	0.72
1:B:110:MSE:CE	1:B:113:TRP:HE3	1.98	0.71
1:B:110:MSE:HE2	1:B:114:TYR:HE1	1.54	0.71
1:A:86:LEU:O	1:A:90:GLU:HG2	1.92	0.70
1:B:77:VAL:HG22	1:B:124:GLN:HG3	1.75	0.69
1:A:77:VAL:HG22	1:A:124:GLN:HG3	1.75	0.68
1:B:270:GLU:HG2	3:B:853:HOH:O	1.96	0.66
1:B:168:GLY:O	1:B:172:GLU:HG3	1.99	0.63
1:A:110:MSE:HE3	1:A:114:TYR:CE1	2.36	0.61
1:B:100:VAL:HG23	1:B:101:LEU:HD12	1.82	0.61
1:A:59:TYR:CD2	1:A:60:ASN:OD1	2.56	0.59
1:A:76:LEU:HD12	1:A:134:ILE:HD11	1.84	0.59
1:B:110:MSE:CE	1:B:113:TRP:CE3	2.79	0.58
1:A:75:LYS:HE3	3:A:783:HOH:O	2.02	0.58
1:B:110:MSE:HE3	1:B:110:MSE:HA	1.84	0.57
1:A:110:MSE:HE2	1:A:210:VAL:HG12	1.88	0.55
1:A:92:TYR:OH	1:A:116:LYS:NZ	2.40	0.52
1:B:254:HIS:HD2	3:B:855:HOH:O	1.92	0.52
1:A:213:LYS:HD3	1:A:245:MSE:HG2	1.93	0.50
1:A:192:MSE:HB3	1:A:200:LEU:HD13	1.94	0.50
1:A:242:ASP:HB3	1:A:245:MSE:HE2	1.94	0.49
1:A:25:ASN:HB3	1:A:28:ARG:HB3	1.94	0.49
1:B:76:LEU:HD12	1:B:134:ILE:HD11	1.94	0.48

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A 4 1		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:A:59:TYR:CE2	1:A:60:ASN:OD1	2.67	0.48
1:A:133:GLU:HG3	3:A:655:HOH:O	2.13	0.47
1:B:197:ASN:HB3	3:B:780:HOH:O	2.15	0.47
1:A:128:LYS:CE	3:A:634:HOH:O	2.36	0.46
1:A:59:TYR:O	1:A:62:LYS:N	2.39	0.46
1:A:119:GLY:O	1:A:123:GLU:HG3	2.16	0.45
1:B:62:LYS:HA	1:B:62:LYS:HD2	1.73	0.45
1:A:9:HIS:HB2	1:A:12:MSE:HE2	1.99	0.45
1:B:171:LEU:HD23	1:B:171:LEU:C	2.37	0.44
1:A:95:ILE:HG21	1:A:109:TYR:CG	2.53	0.44
1:A:264:ARG:NH1	1:A:267:GLU:OE2	2.50	0.44
1:B:95:ILE:HG21	1:B:109:TYR:CG	2.53	0.43
1:A:58:SER:HB3	3:A:723:HOH:O	2.18	0.43
1:B:53:THR:O	1:B:143:LYS:CE	2.67	0.43
1:A:28:ARG:O	1:A:31:GLU:HG2	2.19	0.42
1:B:20:SER:HB2	1:B:281:VAL:O	2.19	0.42
1:A:62:LYS:HB3	1:A:62:LYS:HE3	1.86	0.42
1:A:126:ILE:HA	1:A:127:PRO:HD3	1.90	0.41
1:B:140:VAL:O	1:B:141:MSE:HG2	2.20	0.41
1:A:20:SER:HB2	1:A:281:VAL:O	2.21	0.41
1:B:59:TYR:O	1:B:62:LYS:N	2.39	0.41
1:B:49:BFD:F2	1:B:51:ASP:HB2	2.11	0.40
1:A:140:VAL:O	1:A:141:MSE:HG2	2.22	0.40
1:B:163:PHE:HE1	1:B:208:ILE:HD13	1.86	0.40

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	A	288/297 (97%)	277 (96%)	10 (4%)	1 (0%)	41 50

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Mol	Chain	Analysed Favoured Allowed		Outliers	Perce	ntiles	
1	В	288/297 (97%)	279 (97%)	8 (3%)	1 (0%)	41	50
All	All	576/594 (97%)	556 (96%)	18 (3%)	2 (0%)	41	50

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	В	222	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	Rotameric Outliers	
1	A	$259/257 \ (101\%)$	252 (97%)	7 (3%)	44 61
1	В	259/257 (101%)	253 (98%)	6 (2%)	50 67
All	All	518/514 (101%)	505 (98%)	13 (2%)	47 65

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	28	ARG
1	A	141	MSE
1	A	226	GLN
1	A	236	LEU
1	A	239	SER
1	A	266	ASP
1	В	25	ASN
1	В	58	SER
1	В	110	MSE
1	В	141	MSE
1	В	148	ASN
1	В	181	TYR



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	В	9	HIS
1	В	60	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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 Re	Peg	Link	В	ond leng	$\operatorname{gths}$	Bond angles				
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	BFD	В	49	2,1	8,11,12	1.42	1 (12%)	3,15,17	1.42	0
1	BFD	A	49	2,1	8,11,12	1.29	2 (25%)	3,15,17	1.46	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
1	BFD	В	49	2,1	-	0/5/11/13	-
1	BFD	A	49	2,1	-	0/5/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	В	49	BFD	F3-BE	-2.42	1.48	1.54
1	A	49	BFD	F2-BE	-2.26	1.48	1.54
1	A	49	BFD	F3-BE	-2.23	1.48	1.54



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	49	BFD	1	0

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 $>$	#R5	$\mathbf{SRZ}$	· <b>2</b>	$OWAB(A^2)$	Q < 0.9
1	A	282/297 (94%)	-0.28	1 (0%)	92	95	31, 37, 44, 53	1 (0%)
1	В	$282/297 \ (94\%)$	-0.31	1 (0%)	92	95	30, 37, 45, 53	1 (0%)
All	All	564/594 (94%)	-0.30	2 (0%)	92	95	30, 37, 45, 53	2 (0%)

#### All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	TYR	2.0
1	В	60	ASN	2.0

### 6.2 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	BFD	В	49	12/13	0.94	0.13	30,34,36,39	0
1	BFD	A	49	12/13	0.96	0.10	33,36,38,39	0

### 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	MG	В	602	1/1	0.92	0.05	33,33,33,33	0
2	MG	A	601	1/1	0.94	0.04	28,28,28,28	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

