



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:15 PM EDT

PDB ID : 4AVF  
Title : Crystal structure of Pseudomonas aeruginosa inosine 5'-monophosphate dehydrogenase  
Authors : McMahon, S.A.; Moynie, L.; Liu, H.; Duthie, F.; Naismith, J.H.  
Deposited on : 2012-05-25  
Resolution : 2.23 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9461 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 INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2271	1424	405	430	12			
1	B	316	Total	C	N	O	S	0	1	0
			2285	1438	405	429	13			
1	C	314	Total	C	N	O	S	0	0	0
			2266	1426	402	426	12			
1	D	315	Total	C	N	O	S	0	0	0
			2279	1431	406	430	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q9HXM5
B	0	GLY	-	expression tag	UNP Q9HXM5
C	0	GLY	-	expression tag	UNP Q9HXM5
D	0	GLY	-	expression tag	UNP Q9HXM5

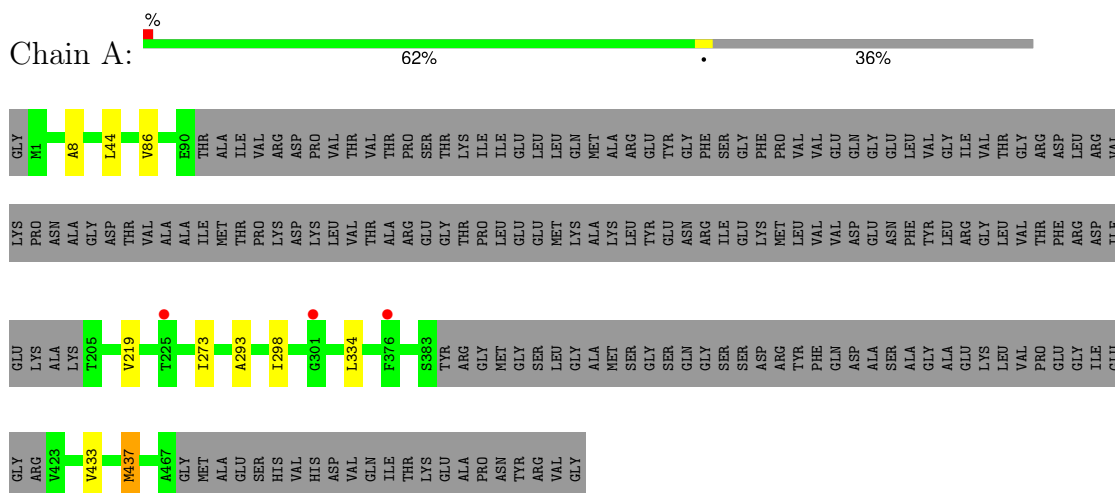
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		
2	B	80	Total	O	0	0
			80	80		
2	C	93	Total	O	0	0
			93	93		
2	D	77	Total	O	0	0
			77	77		

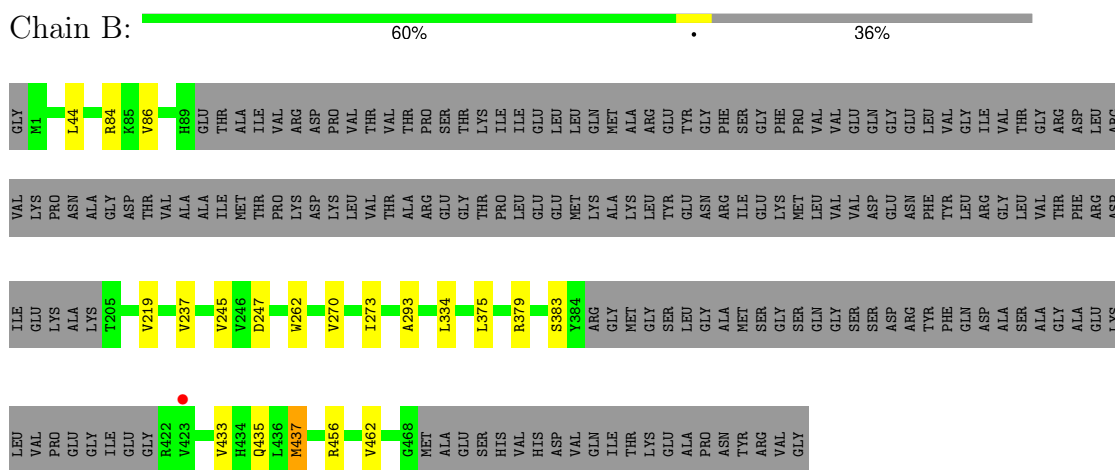
### 3 Residue-property plots

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.

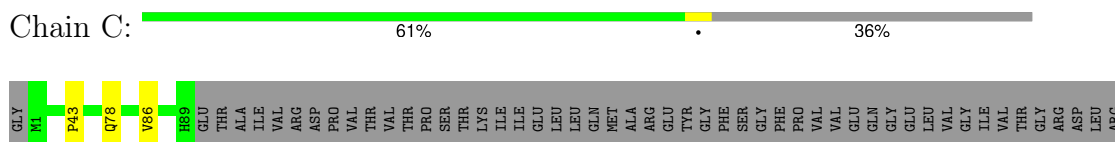
- Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE



- Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE



● Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE



VAL  
LYS  
PRO  
ASN  
ALA  
LYS  
GLY  
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THR  
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ALA  
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ILE  
GLU  
LYS  
ALA  
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T205  
V219  
V245  
D247  
I273  
A293  
I298  
G301  
S302  
I303  
L334  
Y384  
ARG  
GLY  
MET  
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ILE  
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V423  
M437  
A467  
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ALA  
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● Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE



GLY  
HI  
L44  
V86  
H69  
GLU  
THR  
ALA  
MET  
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THR  
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GLU

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T205  
G215  
R216  
V219  
V262  
I273  
E298  
A293  
G299  
C304  
L334  
E372  
F376  
Q377  
Y384  
ARG  
GLY  
MET  
GLY  
SER  
SER  
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V423  
V433  
M437  
G468  
MET  
ALA  
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GLY

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.59Å 116.59Å 259.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.33 – 2.23 106.33 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.9 (106.33-2.23) 99.9 (106.33-2.23)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.179 , 0.200 0.187 , 0.203	Depositor DCC
$R_{free}$ test set	4397 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/2297	0.64	0/3105
1	B	0.52	1/2313 (0.0%)	0.65	0/3126
1	C	0.51	0/2294	0.63	0/3102
1	D	0.51	1/2307 (0.0%)	0.64	0/3119
All	All	0.51	2/9211 (0.0%)	0.64	0/12452

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	TRP	CD2-CE2	5.28	1.47	1.41
1	D	262	TRP	CD2-CE2	5.21	1.47	1.41

There are no bond angle outliers.

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	2271	0	2327	9	0
1	B	2285	0	2343	14	0
1	C	2266	0	2323	7	0
1	D	2279	0	2336	10	0
2	A	110	0	0	0	0
2	B	80	0	0	2	0
2	C	93	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	77	0	0	1	0
All	All	9461	0	9329	36	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 (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB2	1:B:462:VAL:HG21	1.46	0.95
1:B:237:VAL:HG22	1:B:270[A]:VAL:HG21	1.71	0.71
1:A:8:ALA:CB	1:B:462:VAL:HG21	2.22	0.70
1:A:8:ALA:HB2	1:B:462:VAL:CG2	2.21	0.70
1:D:44:LEU:HD12	1:D:437:MET:HE3	1.77	0.66
1:A:433:VAL:HG13	1:A:437:MET:CE	2.28	0.64
1:D:44:LEU:CD1	1:D:437:MET:HE3	2.30	0.62
1:B:84:ARG:NH1	2:B:2033:HOH:O	2.22	0.59
1:D:273:ILE:HG12	1:D:293:ALA:HB3	1.87	0.57
1:A:44:LEU:HD12	1:A:437:MET:HE3	1.88	0.55
1:C:86:VAL:HG11	1:C:219:VAL:HB	1.90	0.54
1:A:433:VAL:HG13	1:A:437:MET:HE3	1.89	0.54
1:C:423:VAL:O	1:C:423:VAL:HG13	2.08	0.53
1:B:86:VAL:HG11	1:B:219:VAL:HB	1.91	0.53
1:C:302:SER:HB2	1:C:303:ILE:HD12	1.90	0.53
1:B:433:VAL:HG13	1:B:437:MET:HE3	1.92	0.52
1:B:433:VAL:O	1:B:437:MET:HE2	2.11	0.50
1:B:375:LEU:HD12	1:B:379:ARG:O	2.12	0.49
1:D:216:ARG:NH2	2:D:2038:HOH:O	2.46	0.48
1:B:245:VAL:HG12	1:B:247:ASP:HB2	1.97	0.47
1:D:86:VAL:HG11	1:D:219:VAL:HB	1.97	0.47
1:D:433:VAL:O	1:D:437:MET:HE2	2.16	0.46
1:D:433:VAL:HG13	1:D:437:MET:HE3	1.99	0.45
1:D:44:LEU:HD11	1:D:437:MET:CE	2.46	0.45
1:B:44:LEU:HD12	1:B:437:MET:HE3	1.99	0.44
1:A:273:ILE:HG12	1:A:293:ALA:HB3	2.00	0.43
1:C:43:PRO:HD2	1:C:437:MET:HE2	2.00	0.43
1:A:86:VAL:HG11	1:A:219:VAL:HB	2.00	0.43
1:B:273:ILE:HG12	1:B:293:ALA:HB3	2.01	0.43
1:C:78:GLN:HG3	2:C:2041:HOH:O	2.18	0.43
1:C:245:VAL:HG12	1:C:247:ASP:HB2	2.00	0.43
1:B:456:ARG:NH1	2:B:2078:HOH:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:GLY:HA2	1:D:304:CYS:SG	2.59	0.43
1:C:273:ILE:HG12	1:C:293:ALA:HB3	1.99	0.42
1:A:8:ALA:CB	1:B:462:VAL:CG2	2.90	0.42
1:D:433:VAL:HG13	1:D:437:MET:CE	2.50	0.41

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	308/490 (63%)	301 (98%)	7 (2%)	0	100	100
1	B	311/490 (64%)	304 (98%)	7 (2%)	0	100	100
1	C	308/490 (63%)	301 (98%)	7 (2%)	0	100	100
1	D	309/490 (63%)	304 (98%)	5 (2%)	0	100	100
All	All	1236/1960 (63%)	1210 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Percentiles	
1	A	227/373 (61%)	224 (99%)	3 (1%)	69	76
1	B	226/373 (61%)	222 (98%)	4 (2%)	59	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	225/373 (60%)	222 (99%)	3 (1%)	69	76
1	D	227/373 (61%)	224 (99%)	3 (1%)	69	76
All	All	905/1492 (61%)	892 (99%)	13 (1%)	67	74

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

Mol	Chain	Res	Type
1	A	298	ILE
1	A	334	LEU
1	A	437	MET
1	B	334	LEU
1	B	383	SER
1	B	435	GLN
1	B	437	MET
1	C	298	ILE
1	C	334	LEU
1	C	437	MET
1	D	304	CYS
1	D	334	LEU
1	D	437	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	435	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	314/490 (64%)	-0.13	3 (0%) 82 83	44, 58, 85, 110	0
1	B	316/490 (64%)	-0.12	1 (0%) 94 94	47, 59, 88, 106	0
1	C	314/490 (64%)	-0.12	2 (0%) 89 89	44, 59, 83, 108	0
1	D	315/490 (64%)	-0.09	5 (1%) 72 73	46, 61, 89, 111	0
All	All	1259/1960 (64%)	-0.12	11 (0%) 84 84	44, 59, 87, 111	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	GLY	4.2
1	A	301	GLY	3.5
1	C	303	ILE	3.2
1	D	377	GLN	2.6
1	D	376	PHE	2.6
1	B	423	VAL	2.5
1	A	376	PHE	2.4
1	D	372	GLU	2.2
1	A	225	THR	2.1
1	D	215	GLY	2.1
1	D	288	GLU	2.1

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.