



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:51 PM GMT

PDB ID : 1ME7  
Title : Inosine Monophosphate Dehydrogenase (IMPDH) From Tritrichomonas Foetus with RVP and MOA bound  
Authors : Prosise, G.L.; Wu, J.; Luecke, H.  
Deposited on : 2002-08-08  
Resolution : 2.15 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

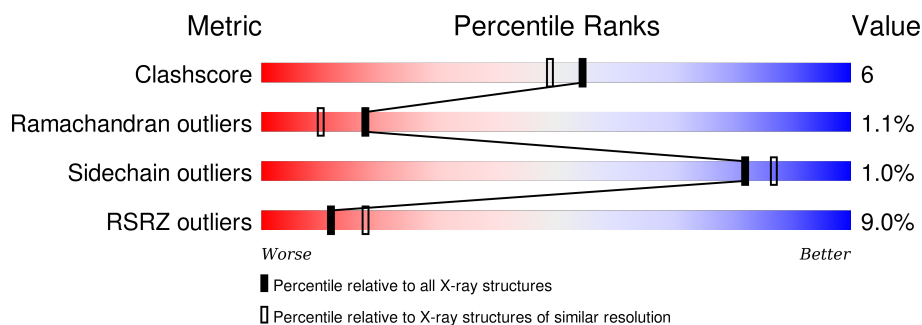
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	503	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2948 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	365	Total	C	N	O	S	0	0	0
			2782	1761	474	531	16			

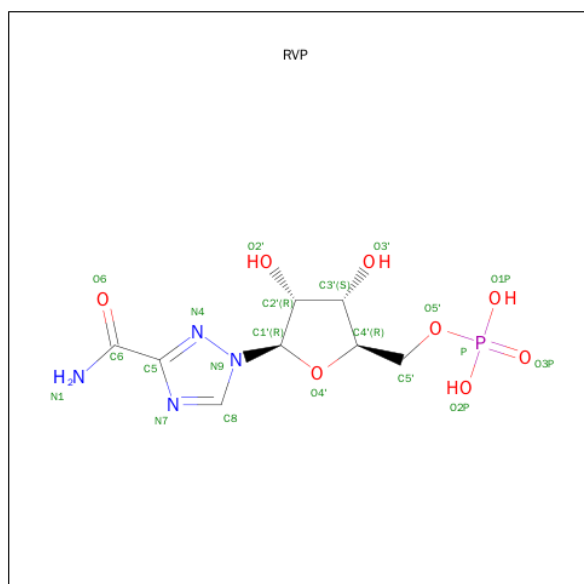
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

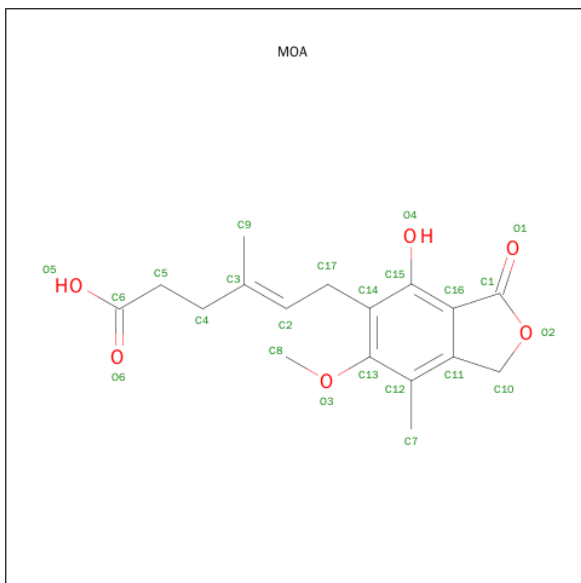
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is RIBAVIRIN MONOPHOSPHATE (three-letter code: RVP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			21	8	4	8	1		

- Molecule 5 is MYCOPHENOLIC ACID (three-letter code: MOA) (formula:  $C_{17}H_{20}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	17	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.07Å 155.07Å 155.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.15 49.04 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.04-2.15) 86.2 (49.04-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.264 0.245 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 33134 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, RVP, MOA

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	0.33	0/2830	0.58	0/3818

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2782	0	2769	36	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	21	0	11	0	0
5	A	23	0	19	0	0
6	A	120	0	0	1	0
All	All	2948	0	2799	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 6.

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:248:PRO:O	1:A:252:GLU:HG2	1.68	0.94
1:A:41:GLN:HE22	1:A:351:ILE:HG12	1.34	0.90
1:A:41:GLN:NE2	1:A:351:ILE:HG12	1.99	0.75
1:A:344:LYS:O	1:A:348:GLU:HG3	1.90	0.72
1:A:362:VAL:H	1:A:366:HIS:HD2	1.39	0.70
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.81	0.63
1:A:225:LEU:HG	1:A:233:LEU:HD12	1.81	0.61
1:A:280:LYS:O	1:A:280:LYS:HD3	2.04	0.57
1:A:320:ILE:H	1:A:324:GLN:HE22	1.54	0.56
1:A:221:CYS:O	1:A:224:GLU:HG2	2.08	0.54
1:A:397:ILE:HG22	1:A:398:ASN:ND2	2.22	0.54
1:A:284:LYS:HD2	1:A:284:LYS:N	2.24	0.53
1:A:443:LEU:C	1:A:443:LEU:HD23	2.31	0.51
1:A:482:SER:O	1:A:483:ILE:HB	2.10	0.51
1:A:356:CYS:HB2	1:A:377:PHE:CE2	2.46	0.50
1:A:371:LEU:O	1:A:470:GLN:HG2	2.11	0.50
1:A:322:ARG:C	1:A:324:GLN:H	2.17	0.48
1:A:479:SER:OG	1:A:482:SER:HB3	2.15	0.47
1:A:72:ALA:HA	1:A:76:GLY:O	2.15	0.46
1:A:318:ILE:HG22	1:A:433:VAL:HG23	1.96	0.46
1:A:466:ILE:O	1:A:470:GLN:HG3	2.15	0.46
1:A:320:ILE:HG21	1:A:323:GLU:OE1	2.16	0.45
1:A:362:VAL:H	1:A:366:HIS:CD2	2.28	0.44
1:A:409:GLY:O	1:A:431:GLU:HB2	2.17	0.44
1:A:229:GLN:OE1	1:A:231:ARG:NH1	2.51	0.44
1:A:103:PHE:C	1:A:103:PHE:CD1	2.91	0.44
1:A:60:GLN:HG3	1:A:408:GLU:OE2	2.17	0.44
1:A:280:LYS:HD2	1:A:281:TYR:CZ	2.53	0.43
1:A:27:ILE:HG12	1:A:30:ASN:ND2	2.33	0.43
1:A:380:LEU:N	1:A:380:LEU:HD12	2.33	0.43
1:A:220:VAL:HG12	1:A:220:VAL:O	2.20	0.42
1:A:33:LEU:HB3	1:A:53:PRO:HD3	2.02	0.42
1:A:413:ALA:C	1:A:415:ASN:H	2.24	0.41
1:A:11:THR:HB	6:A:929:HOH:O	2.20	0.41
1:A:482:SER:O	1:A:483:ILE:CB	2.70	0.40
1:A:89:GLN:HG2	1:A:250:LEU:HD21	2.04	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	359/503 (71%)	336 (94%)	19 (5%)	4 (1%)	17	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	ILE
1	A	414	ARG
1	A	323	GLU
1	A	104	VAL

### 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	297/424 (70%)	294 (99%)	3 (1%)	82	87

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

Mol	Chain	Res	Type
1	A	266	PHE
1	A	415	ASN
1	A	481	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	30	ASN
1	A	41	GLN
1	A	324	GLN
1	A	331	GLN
1	A	366	HIS
1	A	398	ASN
1	A	415	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	MOA	A	600	-	21,24,24	1.74	5 (23%)	30,34,34	1.93	9 (30%)
4	RVP	A	602	-	18,22,22	4.28	5 (27%)	21,33,33	1.96	6 (28%)

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
5	MOA	A	600	-	-	0/10/21/21	0/2/2/2
4	RVP	A	602	-	-	0/6/30/30	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	RVP	C5-C6	-15.52	1.46	1.53
4	A	602	RVP	C8-N7	-3.07	1.29	1.35
5	A	600	MOA	O2-C1	-2.21	1.33	1.36
4	A	602	RVP	O4'-C1'	2.41	1.44	1.41
5	A	600	MOA	C15-C14	2.84	1.44	1.40
5	A	600	MOA	C11-C12	3.02	1.45	1.40
5	A	600	MOA	C13-C12	3.09	1.45	1.39
5	A	600	MOA	C13-C14	3.55	1.45	1.39
4	A	602	RVP	C8-N9	5.21	1.39	1.33
4	A	602	RVP	C6-N1	5.80	1.44	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	RVP	N4-C5-N7	-5.88	110.16	114.88
5	A	600	MOA	O2-C1-C16	-3.25	105.52	108.31
5	A	600	MOA	C4-C3-C2	-2.78	115.77	121.05
4	A	602	RVP	C8-N9-N4	-2.77	105.15	108.84
4	A	602	RVP	O6-C6-N1	-2.61	118.92	122.59
5	A	600	MOA	O2-C10-C11	-2.50	102.08	104.69
5	A	600	MOA	C14-C13-C12	-2.27	119.79	122.80
4	A	602	RVP	C4'-O4'-C1'	-2.24	107.26	109.72
5	A	600	MOA	C17-C14-C15	-2.12	118.31	121.01
5	A	600	MOA	C15-C14-C13	2.15	120.80	117.90
4	A	602	RVP	O6-C6-C5	2.69	126.68	119.69
4	A	602	RVP	O1P-P-O5'	2.88	114.84	106.56
5	A	600	MOA	O2-C1-O1	2.99	124.03	121.05
5	A	600	MOA	C9-C3-C4	3.06	120.08	115.41
5	A	600	MOA	C10-O2-C1	6.59	115.06	110.59

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

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

### 6.1 Protein, DNA and RNA chains

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	365/503 (72%)	0.42	33 (9%) 12 18	27, 40, 80, 102	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	11.1
1	A	320	ILE	8.5
1	A	105	VAL	8.4
1	A	103	PHE	7.5
1	A	102	GLY	6.6
1	A	106	SER	6.3
1	A	414	ARG	6.1
1	A	220	VAL	5.7
1	A	415	ASN	5.6
1	A	107	ASP	5.4
1	A	101	ALA	4.9
1	A	487	GLY	4.9
1	A	486	GLY	4.8
1	A	431	GLU	4.6
1	A	222	HIS	4.4
1	A	483	ILE	4.2
1	A	484	VAL	4.1
1	A	416	TRP	4.0
1	A	490	ASP	3.8
1	A	315	GLY	3.2
1	A	488	ALA	3.2
1	A	324	GLN	3.2
1	A	481	VAL	2.9
1	A	323	GLU	2.8
1	A	413	ALA	2.8
1	A	491	VAL	2.8
1	A	322	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	321	THR	2.7
1	A	318	ILE	2.4
1	A	319	CYS	2.1
1	A	94	HIS	2.0
1	A	221	CYS	2.0
1	A	480	SER	2.0

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MOA	A	600	23/23	0.74	0.38	1.99	44,46,52,53	23
2	NA	A	901	1/1	0.83	0.31	0.27	69,69,69,69	0
4	RVP	A	602	21/21	0.96	0.10	-0.60	35,40,41,42	0
3	K	A	900	1/1	0.98	0.09	-1.29	36,36,36,36	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.