

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 11:04 pm BST

PDB ID	:	1JR1
Title	:	Crystal structure of Inosine Monophosphate Dehydrogenase in complex with
		Mycophenolic Acid
Authors	:	Sintchak, M.D.; Fleming, M.A.; Futer, O.; Raybuck, S.A.; Chambers, S.P.;
		Caron, P.R.; Murcko, M.A.; Wilson, K.P.
Deposited on	:	2001-08-09
Resolution	:	2.60 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 following versions of software and data (see references (1)) were used in the production of this report:

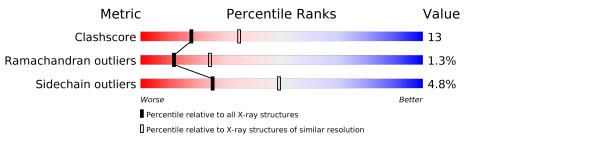
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455(2.60-2.60)
Sidechain outliers	138945	3455(2.60-2.60)

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 >=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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	А	514	60%		22%	• 15%		
1	В	514	51%	19%	•	28%		



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6296 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.

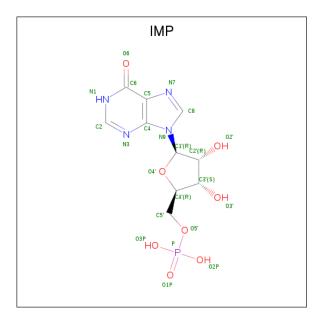
• Molecule 1 is a protein called Inosine-5'-Monophosphate Dehydrogenase 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	436	Total	С	Ν	Ο	S	0	0	0
		430	3236	2041	560	616	19	0		
1	В	368	Total	С	Ν	Ο	S	0	0	0
	D	308	2764	1750	471	525	18	0		

• Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total K 1 1	0	0
2	А	1	Total K 1 1	0	0

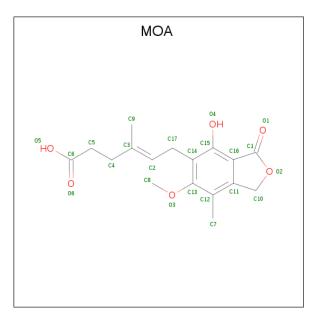
• Molecule 3 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	3 A	1	Total	С	Ν	Ο	Р	0	0
0		1	23	10	4	8	1	0	
2	р	1	Total	С	Ν	Ο	Р	0	0
0	D		23	10	4	8	1	U	U

• Molecule 4 is MYCOPHENOLIC ACID (three-letter code: MOA) (formula: $C_{17}H_{20}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C O 23 17 6	0	0
4	В	1	Total C O 23 17 6	0	0

• Molecule 5 is water.

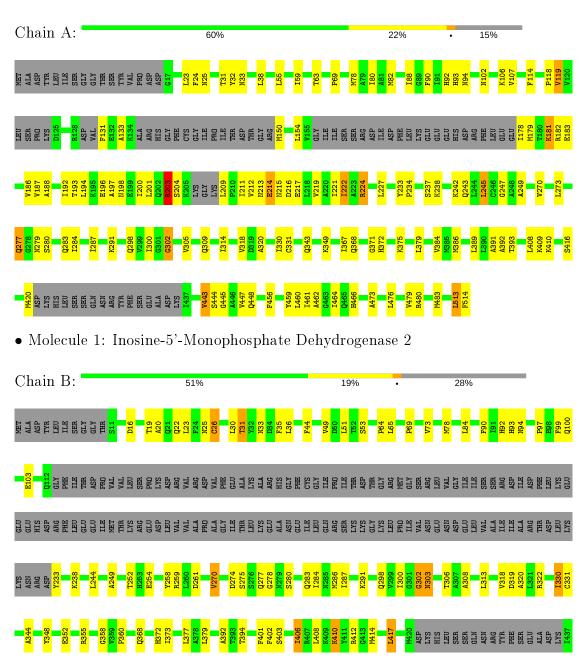
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	122	Total O 122 122	0	0
5	В	80	Total O 80 80	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. Residues are colorcoded 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. 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.

Note EDS was not executed.



• Molecule 1: Inosine-5'-Monophosphate Dehydrogenase 2



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 4	Depositor	
Cell constants	110.60Å 110.60Å 111.00Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	8.00 - 2.60	Depositor	
% Data completeness	(Not available) (8.00-2.60)	Depositor	
(in resolution range)	(100 available) (0.00 2.00)	Depositor	
R_{merge}	(Not available)	Depositor	
R _{sym}	5.20	Depositor	
Refinement program	X-PLOR 3.851	Depositor	
R, R_{free}	0.217 , 0.285	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	6296	wwPDB-VP	
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP	



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: IMP, K, 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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.37	0/3276	0.62	1/4417~(0.0%)	
1	В	0.38	0/2807	0.62	0/3787	
All	All	0.37	0/6083	0.62	1/8204~(0.0%)	

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	118	PRO	N-CA-CB	5.75	110.20	103.30

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	А	3236	0	3234	89	0
1	В	2764	0	2794	75	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	23	0	10	0	0
3	В	23	0	11	2	0
4	А	23	0	19	0	0
4	В	23	0	19	0	0

Continued on next page...



Continued from previous page...

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 13.

The worst 5 of 164 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:B:417:LEU:HD23	1:B:440:ALA:HB2	1.47	0.96
1:A:392:ALA:HB2	1:A:447:VAL:HG23	1.51	0.92
1:A:283:GLN:HE22	1:A:302:GLY:HA3	1.43	0.84
1:B:100:GLN:OE1	1:B:259:ARG:HD2	1.80	0.82
1:A:368:GLN:H	1:A:372:HIS:HD2	1.27	0.80

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	А	422/514~(82%)	386~(92%)	28~(7%)	8 (2%)	8 15
1	В	362/514~(70%)	338~(93%)	22~(6%)	2(1%)	25 47
All	All	784/1028~(76%)	724 (92%)	50 (6%)	10 (1%)	12 24

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	119	VAL
1	А	179	MET

Continued on next page...



Chain Non-H H(model) H(added) Clashes Symm-Clashes Mol 51220 А 0 0 1 5В 0 3 0 0 80 All All 6296 0 6087 1640

 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	А	214	GLU
1	В	254	GLU
1	А	183	GLU

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	А	333/420~(79%)	318~(96%)	15~(4%)	27 52
1	В	292/420~(70%)	277~(95%)	15~(5%)	24 46
All	All	625/840~(74%)	595~(95%)	30~(5%)	25 49

 $5~{\rm of}~30$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	483	MET
1	В	26	CYS
1	В	483	MET
1	В	16	ASP
1	В	30	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	372	HIS
1	А	466	HIS
1	В	285	ASN
1	А	343	GLN
1	В	312	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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	Mol Type Chain		Dog	Bos	Bos	Dec	Dec	Dog	Dog	Res	Pog	Link	Bond lengths				Bond angles		
	Type	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2									
4	MOA	А	1332	-	21,24,24	1.08	2 (9%)	31,34,34	1.97	<mark>9 (29%)</mark>									
3	IMP	В	1332	-	21,25,25	1.52	5 (23%)	23,38,38	2.06	2 (8%)									
4	MOA	В	1333	-	21,24,24	1.46	3 (14%)	31,34,34	1.85	8 (25%)									
3	IMP	А	1331	1	21,25,25	1.59	4 (19%)	23,38,38	2.08	<mark>5 (21%)</mark>									

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
4	MOA	А	1332	-	-	0/10/21/21	0/2/2/2
3	IMP	В	1332	-	-	0/6/26/26	0/3/3/3
4	MOA	В	1333	-	-	0/10/21/21	0/2/2/2
3	IMP	А	1331	1	-	0/6/26/26	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	А	1331	IMP	C2-N1	5.11	1.43	1.33
3	В	1332	IMP	C2-N1	3.78	1.40	1.33

Continued on next page...



001000											
Mol	Chain	\mathbf{Res}	Type	Atoms		${ m Observed}({ m \AA})$	Ideal(Å)				
4	В	1333	MOA	O2-C10	3.43	1.49	1.45				
4	В	1333	MOA	C16-C1	3.16	1.52	1.47				
3	В	1332	IMP	C5-C4	2.98	1.48	1.40				

Continued from previous page...

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	1332	IMP	C2-N1-C6	6.91	127.46	115.88
3	А	1331	IMP	C2-N1-C6	6.31	126.45	115.88
4	А	1332	MOA	C10-O2-C1	5.76	114.64	110.63
4	В	1333	MOA	C10-O2-C1	5.40	114.39	110.63
3	В	1332	IMP	N3-C2-N1	-5.34	120.33	128.68

There are no chirality outliers.

There are no torsion outliers.

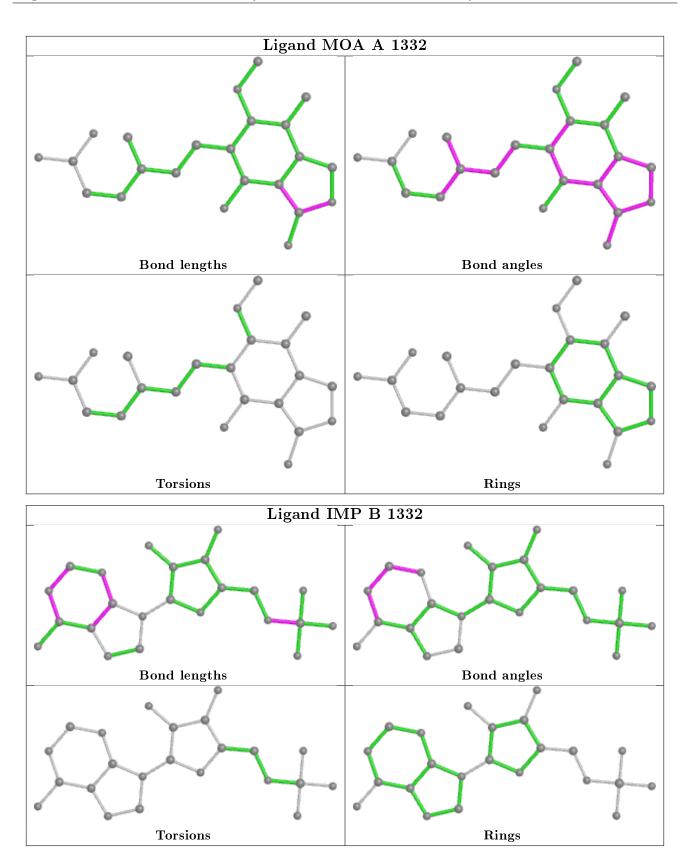
There are no ring outliers.

1 monomer is involved in 2 short contacts:

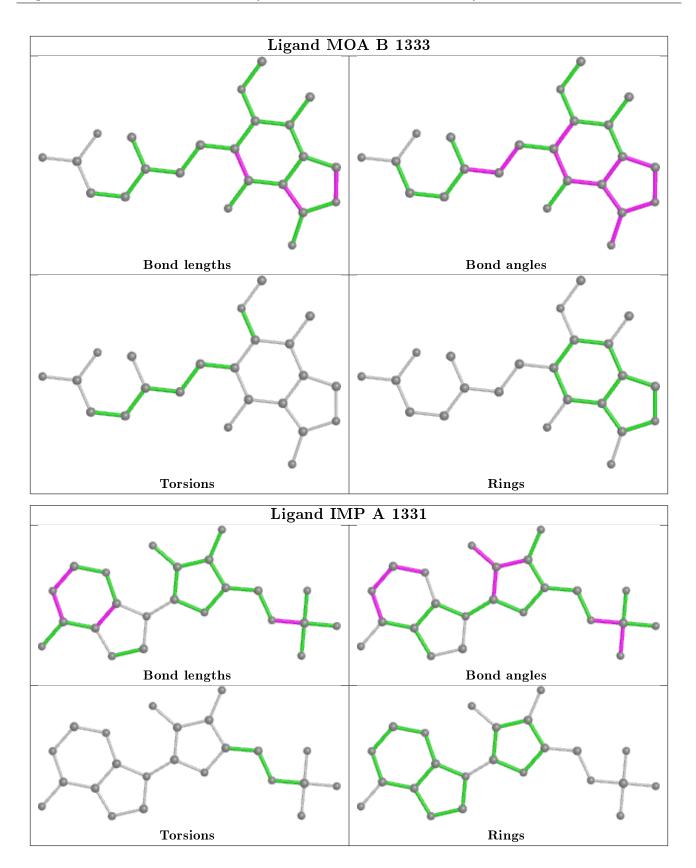
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	1332	IMP	2	0

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.









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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

