



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

• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE



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



GLY	HI	L44	V86	H69	GLU	THR	ALA	ILE	THR	ILE	VAL	ARG	ASP	PRO	VAL	THR	VAL	THR	PRO	THR	ILE	ILE	GLU	LEU	LEU	GLN	MET	ALA	ARG	TYR	GLY	ASN	GLY	PHE	SER	SER	GLY	PHE	PRO	VAL	VAL	GLU	GLN	GLY	GLY	VAL	THR	GLY	ARG	ASP	LEU	THR	ILE	GLY	LYS
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PRO	ASN	ALA	GLY	ASP	THR	VAL	ALA	ILE	MET	THR	PRO	LYS	ASP	LYS	LEU	VAL	THR	ALA	ARG	GLU	GLY	THR	PRO	LEU	GLU	GLY	LYS	ALA	LYS	LEU	TYR	GLY	ASN	ARG	ILE	GLU	LYS	MET	PRO	LEU	VAL	VAL	ASP	GLU	ASN	ASP	PHE	LEU	ARG	GLY	VAL	THR	VAL	THR	PHE	ARG	ASP	ILE	GLU
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LYS	ALA	LYS	T205	G215	R216	V219	V262	I273	E298	A293	G299	C304	L334	E372	F376	Q377	Y384	ARG	GLY	MET	GLY	SER	LEU	GLY	ALA	ALA	MET	SER	LYS	GLY	SER	GLN	GLY	SER	SER	SER	ARG	TYR	PHE	GLN	ASP	ALA	ALA	ALA	GLY	ALA	GLU	LYS	LEU
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VAL	PRO	GLY	ILE	GLY	ARG	V423	V433	M437	G468	MET	ALA	GLU	SER	HIS	VAL	HIS	ASP	VAL	GLN	ILE	THR	LYS	GLU	ALA	PRO	ASN	TYR	ARG	VAL	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	42.5	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

The worst 5 of 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

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
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

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	298	ILE
1	C	334	LEU
1	D	437	MET
1	D	304	CYS
1	D	334	LEU

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 [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](#)

There are no ligands in this entry.

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, 95th 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 ²)	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

The worst 5 of 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

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.