



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:23 am GMT

PDB ID : 1VRD
Title : Crystal structure of Inosine-5'-monophosphate dehydrogenase (TM1347) from THERMOTOGA MARITIMA at 2.18 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-02-22
Resolution : 2.18 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

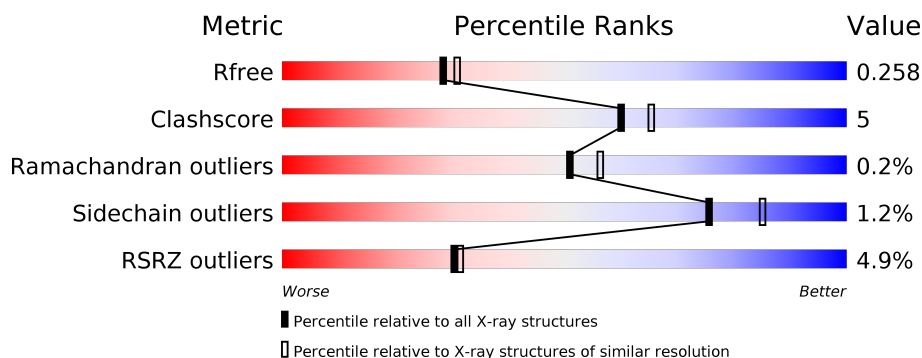
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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))
R_{free}	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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 ≥ 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	494	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>8%</div> <div>35%</div> </div> </div>
1	B	494	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>9%</div> <div>36%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4876 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	321	Total	C	N	O	S	0	0	0
			2363	1490	414	448	11			
1	B	317	Total	C	N	O	S	0	0	0
			2307	1455	404	438	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9X168
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9X168
A	-9	SER	-	LEADER SEQUENCE	UNP Q9X168
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9X168
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9X168
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9X168
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9X168
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9X168
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9X168
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9X168
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9X168
A	0	HIS	-	LEADER SEQUENCE	UNP Q9X168
B	-11	MET	-	LEADER SEQUENCE	UNP Q9X168
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9X168
B	-9	SER	-	LEADER SEQUENCE	UNP Q9X168
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9X168
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9X168
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9X168
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9X168
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9X168
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9X168
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9X168
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9X168
B	0	HIS	-	LEADER SEQUENCE	UNP Q9X168

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	107	Total 107	O 107	0	0
2	B	99	Total 99	O 99	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	120.08Å 120.08Å 144.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.18 46.12 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.2 (46.12-2.18) 94.2 (46.12-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.258 0.218 , 0.258	Depositor DCC
R_{free} test set	2553 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4876	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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	0.71	0/2390	0.75	1/3233 (0.0%)
1	B	0.66	0/2335	0.70	0/3164
All	All	0.69	0/4725	0.73	1/6397 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ARG	NE-CZ-NH1	-5.27	117.67	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	2363	0	2454	26	0
1	B	2307	0	2361	25	0
2	A	107	0	0	3	0
2	B	99	0	0	2	0
All	All	4876	0	4815	50	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 5.

All (50) 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:15:GLN:NE2	1:B:450:LYS:O	2.01	0.93
1:A:198:MET:O	1:A:202:GLU:HG2	1.80	0.81
1:A:442:ARG:HD2	2:A:576:HOH:O	1.80	0.80
1:B:70:LEU:O	1:B:229:ARG:NH2	2.18	0.75
1:B:241:ILE:HD12	1:B:267:LEU:HD21	1.70	0.73
1:B:6:THR:HB	2:B:556:HOH:O	1.95	0.66
1:A:79:VAL:O	1:A:83:LYS:HG2	1.98	0.64
1:B:362:GLY:HA3	1:B:418:LYS:HE2	1.83	0.60
1:A:300:ILE:O	1:A:300:ILE:CG2	2.52	0.58
1:A:356:VAL:HG23	1:A:360:PHE:CE2	2.39	0.57
1:A:33:GLN:HG2	2:A:562:HOH:O	2.05	0.56
1:B:356:VAL:HG23	1:B:360:PHE:CE2	2.42	0.54
1:A:364:GLU:HG3	2:A:584:HOH:O	2.08	0.54
1:B:223:SER:HB2	1:B:224:PRO:HD2	1.90	0.53
1:A:39:PRO:HG3	1:A:444:ILE:HD11	1.89	0.53
1:B:77:ARG:NH1	1:B:81:ILE:HD11	2.25	0.52
1:B:83:LYS:HD3	1:B:216:VAL:HG12	1.93	0.51
1:B:241:ILE:CD1	1:B:267:LEU:HD21	2.41	0.50
1:A:207:ALA:HB1	1:A:215:LEU:HD12	1.93	0.50
1:B:337:ILE:HG22	1:B:359:ILE:HD12	1.95	0.48
1:B:46:ASP:HA	1:B:67:HIS:CD2	2.48	0.48
1:A:21:PRO:O	1:A:24:VAL:HG22	2.14	0.47
1:A:376:ARG:NH2	1:B:376:ARG:HH12	2.13	0.46
1:B:277:PRO:CB	1:B:323:VAL:HG21	2.46	0.46
1:A:223:SER:HB2	1:A:224:PRO:CD	2.46	0.46
1:A:6:THR:HG22	1:A:9:ASP:OD2	2.16	0.46
1:B:53:LEU:HD11	1:B:360:PHE:HB3	1.98	0.45
1:A:241:ILE:HG13	1:A:267:LEU:HD21	1.99	0.45
1:A:58:ALA:HA	1:A:62:GLY:O	2.17	0.45
1:B:296:GLY:N	1:B:297:PRO:HD3	2.32	0.44
1:A:356:VAL:HG23	1:A:360:PHE:CD2	2.53	0.44
1:B:261:LYS:NZ	1:B:267:LEU:O	2.50	0.44
1:A:241:ILE:CG1	1:A:267:LEU:HD21	2.49	0.43
1:B:275:ALA:HB1	1:B:311:VAL:HB	2.00	0.43
1:A:356:VAL:CG2	1:A:360:PHE:CE2	3.02	0.43
1:A:34:ILE:HD11	1:A:268:PRO:HG2	1.99	0.43
1:B:39:PRO:HG3	1:B:444:ILE:HD11	2.01	0.43
1:B:67:HIS:CE1	1:B:70:LEU:HG	2.54	0.43
1:A:67:HIS:CE1	1:A:70:LEU:HG	2.54	0.42
1:B:209:ASP:HB2	2:B:563:HOH:O	2.19	0.42
1:A:272:GLY:HA3	1:A:273:ASN:HA	1.92	0.42
1:B:272:GLY:HA3	1:B:273:ASN:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:VAL:O	1:A:425:VAL:HG23	2.20	0.41
1:B:274:VAL:O	1:B:293:VAL:HA	2.21	0.41
1:A:300:ILE:O	1:A:300:ILE:HG22	2.20	0.41
1:A:41:VAL:O	1:A:355:MET:HA	2.21	0.41
1:B:378:TYR:HB3	1:B:414:MET:HG2	2.03	0.41
1:A:28:THR:HB	1:A:444:ILE:HD12	2.03	0.41
1:B:4:ALA:CB	1:B:312:PRO:HD2	2.51	0.41
1:A:16:TYR:CE2	1:A:18:GLU:HG3	2.56	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	315/494 (64%)	304 (96%)	11 (4%)	0	100	100
1	B	311/494 (63%)	304 (98%)	6 (2%)	1 (0%)	44	47
All	All	626/988 (63%)	608 (97%)	17 (3%)	1 (0%)	51	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	ILE

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	246/405 (61%)	242 (98%)	4 (2%)	68	79
1	B	235/405 (58%)	233 (99%)	2 (1%)	82	90
All	All	481/810 (59%)	475 (99%)	6 (1%)	75	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	35	ARG
1	A	370	THR
1	A	382	ARG
1	B	238	VAL
1	B	415	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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, 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	321/494 (64%)	0.09	10 (3%) 49 50	27, 37, 57, 76	0
1	B	317/494 (64%)	0.24	21 (6%) 19 20	27, 37, 61, 80	0
All	All	638/988 (64%)	0.17	31 (4%) 30 31	27, 37, 60, 80	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	ILE	5.1
1	A	373	TYR	4.7
1	B	414	MET	4.4
1	B	300	ILE	3.7
1	B	373	TYR	3.7
1	A	410	GLY	3.7
1	B	298	GLY	3.7
1	B	384	MET	3.6
1	A	411	ILE	3.2
1	B	375	GLY	3.2
1	A	371	ILE	3.0
1	A	85	THR	3.0
1	A	374	GLN	2.9
1	A	298	GLY	2.9
1	B	51	ALA	2.8
1	B	380	ALA	2.7
1	B	376	ARG	2.7
1	A	375	GLY	2.6
1	B	78	GLN	2.6
1	A	202	GLU	2.6
1	B	411	ILE	2.5
1	B	299	SER	2.4
1	B	199	SER	2.4
1	A	382	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	79	VAL	2.3
1	B	413	GLY	2.2
1	B	75	GLN	2.2
1	B	368	GLY	2.1
1	B	377	LYS	2.1
1	B	410	GLY	2.1
1	B	230	VAL	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 carbohydrates 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.