



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:12 pm BST

PDB ID : 3FYC  
Title : Crystal Structure of Dim1 from the thermophilic archeon, Methanocaldococcus jannaschi  
Authors : Scarsdale, J.N.; Musayev, F.N.; Rife, J.P.  
Deposited on : 2009-01-22  
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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

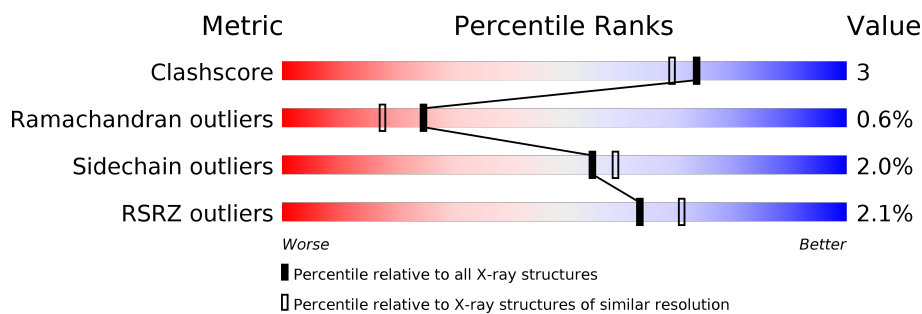
# 1 Overall quality at a glance

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	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 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  $\leq 5\%$ . 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	265	<div> <div>3%</div> <div>88%</div> <div>11%</div> </div>
1	B	265	<div> <div>2%</div> <div>89%</div> <div>10%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4649 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.

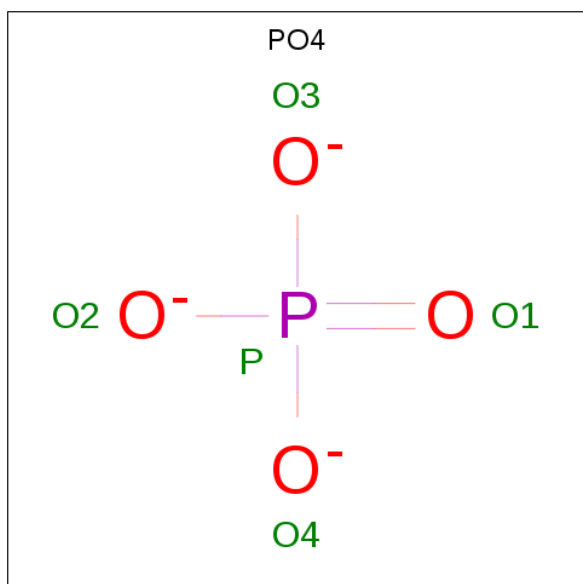
- Molecule 1 is a protein called Probable dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	3	0
			2138	1384	357	392	5			
1	B	265	Total	C	N	O	S	0	4	0
			2169	1400	362	403	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	-	EXPRESSION TAG	UNP Q58435
A	9	ALA	-	EXPRESSION TAG	UNP Q58435
B	8	ALA	-	EXPRESSION TAG	UNP Q58435
B	9	ALA	-	EXPRESSION TAG	UNP Q58435

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



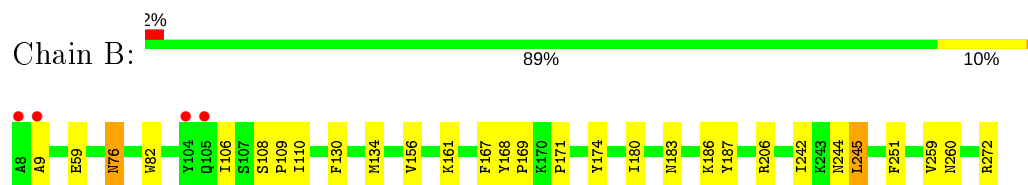
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 10 8 2	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	159	Total O 162 162	0	3
3	B	126	Total O 130 130	0	4

**i**

- Molecule 1: Probable dimethyladenosine transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.38Å 72.27Å 95.88Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	32.00 – 2.15 31.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.9 (32.00-2.15) 94.9 (31.94-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.273 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.39	0/2176	0.55	0/2933
1	B	0.38	0/2207	0.53	1/2976 (0.0%)
All	All	0.39	0/4383	0.54	1/5909 (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	B	245	LEU	CA-CB-CG	6.77	130.87	115.30

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	2138	0	2171	16	0
1	B	2169	0	2203	13	0
2	A	20	0	0	0	0
2	B	30	0	0	0	0
3	A	162	0	0	1	0
3	B	130	0	0	0	0
All	All	4649	0	4374	29	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 3.

All (29) 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:169:PRO:O	1:A:170:LYS:HB3	1.85	0.76
1:A:128:TYR:CE2	1:A:132:LYS:HD2	2.29	0.68
1:A:11[A]:CYS:H	1:A:169:PRO:HD2	1.67	0.60
1:A:161:LYS:HE2	1:A:174:TYR:CD1	2.40	0.57
1:A:65:GLU:N	1:A:66:PRO:HD2	2.20	0.57
1:A:271:ASN:HB2	3:A:407:HOH:O	2.04	0.56
1:A:84:ASP:O	1:A:88:VAL:HG23	2.08	0.53
1:A:140:THR:O	1:A:206:ARG:NH2	2.43	0.51
1:A:84:ASP:HB3	1:A:87:LYS:HB2	1.93	0.49
1:B:59:GLU:O	1:B:82:TRP:HA	2.12	0.48
1:A:206:ARG:HG2	1:A:251:PHE:HB3	1.95	0.48
1:A:121:LEU:HD11	1:A:179:LYS:HG2	1.97	0.46
1:A:165:SER:HA	1:A:170:LYS:HE2	1.98	0.46
1:B:167:PHE:HB2	1:B:171:PRO:HD3	1.96	0.46
1:B:168:TYR:HA	1:B:169:PRO:C	2.37	0.45
1:A:67:TYR:O	1:A:71:LEU:HB2	2.16	0.45
1:B:130:PHE:O	1:B:134:MET:HG3	2.17	0.45
1:B:156:VAL:HG12	1:B:180:ILE:HG12	2.01	0.43
1:A:156:VAL:HG12	1:A:180:ILE:HG12	2.01	0.43
1:A:167:PHE:HB2	1:A:171:PRO:HD3	2.01	0.43
1:A:266:TYR:O	1:A:270:GLN:HG2	2.20	0.41
1:B:76:ASN:H	1:B:76:ASN:HD22	1.69	0.41
1:B:108:SER:HB3	1:B:109:PRO:HD3	2.01	0.41
1:B:106:ILE:O	1:B:110:ILE:HG22	2.20	0.41
1:B:161:LYS:HE2	1:B:174:TYR:CD1	2.55	0.41
1:B:206:ARG:HG2	1:B:251:PHE:HB3	2.03	0.41
1:B:242:ILE:HD12	1:B:242:ILE:C	2.42	0.40
1:B:187:TYR:HB3	1:B:259:VAL:HG11	2.03	0.40
1:B:183:ASN:HB3	1:B:186:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	266/265 (100%)	254 (96%)	9 (3%)	3 (1%)	14	8
1	B	267/265 (101%)	261 (98%)	5 (2%)	1 (0%)	34	29
All	All	533/530 (101%)	515 (97%)	14 (3%)	4 (1%)	25	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	ALA
1	A	11[A]	CYS
1	A	11[B]	CYS
1	A	170	LYS

### 5.3.2 Protein sidechains

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	231/238 (97%)	227 (98%)	4 (2%)	60	65
1	B	237/238 (100%)	232 (98%)	5 (2%)	53	57
All	All	468/476 (98%)	459 (98%)	9 (2%)	55	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	110	ILE

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Mol	Chain	Res	Type
1	A	226	ASP
1	A	244	ASN
1	B	76	ASN
1	B	244	ASN
1	B	245	LEU
1	B	260	ASN
1	B	272	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	ASN
1	B	244	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](#)

10 ligands are modelled in this entry.

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	$\# Z  > 2$
2	PO4	A	1	-	4,4,4	0.88	0	6,6,6	0.42	0
2	PO4	B	4	-	4,4,4	0.89	0	6,6,6	0.41	0
2	PO4	A	2	-	4,4,4	0.89	0	6,6,6	0.54	0
2	PO4	B	273[B]	-	4,4,4	0.89	0	6,6,6	0.40	0
2	PO4	B	273[A]	-	4,4,4	0.92	0	6,6,6	0.46	0
2	PO4	B	7	-	4,4,4	0.90	0	6,6,6	0.41	0
2	PO4	A	3	-	4,4,4	0.87	0	6,6,6	0.43	0
2	PO4	B	6	-	4,4,4	0.85	0	6,6,6	0.50	0
2	PO4	A	273	-	4,4,4	0.87	0	6,6,6	0.46	0
2	PO4	B	5	-	4,4,4	0.89	0	6,6,6	0.41	0

There are no bond length outliers.

There are no bond angle outliers.

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 [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, 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	265/265 (100%)	-0.06	7 (2%) 56 64	23, 34, 51, 64	0
1	B	265/265 (100%)	0.05	4 (1%) 73 79	23, 35, 52, 60	0
All	All	530/530 (100%)	-0.01	11 (2%) 63 71	23, 34, 52, 64	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	5.0
1	A	8	ALA	3.5
1	B	8	ALA	3.3
1	B	9	ALA	3.1
1	A	74	LEU	2.4
1	A	242	ILE	2.4
1	A	10	GLN	2.3
1	A	239	ASN	2.2
1	B	104	TYR	2.1
1	A	66	PRO	2.1
1	B	105	GLN	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	A	1	5/5	0.58	0.34	111,112,112,112	0
2	PO4	B	273[B]	5/5	0.76	0.29	66,66,67,68	5
2	PO4	B	273[A]	5/5	0.76	0.29	45,46,46,47	5
2	PO4	B	7	5/5	0.77	0.20	94,94,95,95	0
2	PO4	A	2	5/5	0.86	0.17	76,77,79,80	0
2	PO4	B	6	5/5	0.87	0.20	81,81,82,84	0
2	PO4	A	3	5/5	0.89	0.18	69,69,71,72	0
2	PO4	B	5	5/5	0.90	0.12	82,82,83,83	0
2	PO4	A	273	5/5	0.92	0.23	68,68,69,69	0
2	PO4	B	4	5/5	0.95	0.11	82,83,83,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.