



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:46 pm BST

PDB ID : 3TMS  
Title : PLASTIC ADAPTATION TOWARD MUTATIONS IN PROTEINS: STRUCTURAL COMPARISON OF THYMIDYLATE SYNTHASES  
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Deposited on : 1991-09-19  
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

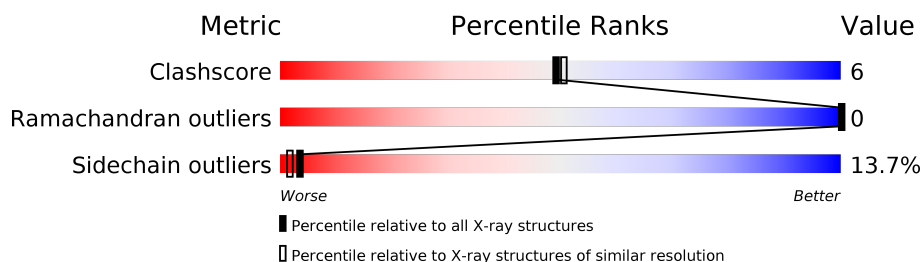
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	265	-	X	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2166 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 THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2150	1374	371	393	12			

- 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	0	0
			5	4	1		

- Molecule 3 is water.

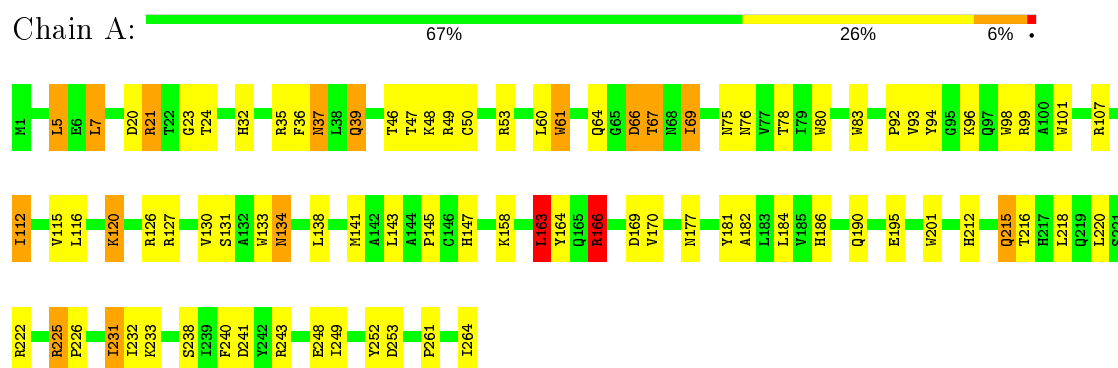
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		

### 3 Residue-property plots

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 color-coded 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: THYMIDYLATE SYNTHASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.00 Å   133.00 Å   133.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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: 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	1.01	2/2210 (0.1%)	1.89	54/3000 (1.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	SER	CA-CB	-5.45	1.44	1.52
1	A	83	TRP	CG-CD2	-5.38	1.34	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH2	20.86	130.73	120.30
1	A	21	ARG	NE-CZ-NH1	-12.39	114.10	120.30
1	A	21	ARG	NE-CZ-NH2	11.88	126.24	120.30
1	A	166	ARG	NE-CZ-NH1	-10.43	115.08	120.30
1	A	35	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	A	243	ARG	NE-CZ-NH2	9.77	125.18	120.30
1	A	201	TRP	CD1-CG-CD2	9.71	114.07	106.30
1	A	83	TRP	CD1-CG-CD2	9.36	113.79	106.30
1	A	133	TRP	CE2-CD2-CG	-8.87	100.21	107.30
1	A	243	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	A	133	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	A	252	TYR	CB-CG-CD2	-8.11	116.13	121.00
1	A	127	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	A	80	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	A	61	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	A	201	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	A	83	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	94	TYR	CB-CG-CD2	-7.77	116.33	121.00
1	A	222	ARG	NE-CZ-NH2	7.69	124.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	TRP	CG-CD2-CE3	7.57	140.71	133.90
1	A	61	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	98	TRP	CG-CD2-CE3	7.22	140.40	133.90
1	A	201	TRP	CG-CD1-NE1	-7.21	102.89	110.10
1	A	201	TRP	CB-CG-CD1	-7.20	117.64	127.00
1	A	107	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	98	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	98	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	A	101	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	170	VAL	CG1-CB-CG2	-6.80	100.02	110.90
1	A	37	ASN	CB-CG-ND2	6.72	132.83	116.70
1	A	101	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	A	126	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	A	233	LYS	N-CA-CB	-6.53	98.84	110.60
1	A	133	TRP	CG-CD2-CE3	6.53	139.77	133.90
1	A	80	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	A	169	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	164	TYR	CB-CG-CD1	-6.14	117.31	121.00
1	A	78	THR	N-CA-CB	-5.84	99.20	110.30
1	A	83	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	A	169	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	36	PHE	CB-CG-CD1	-5.69	116.82	120.80
1	A	115	VAL	CA-CB-CG2	-5.68	102.38	110.90
1	A	101	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	A	233	LYS	CA-CB-CG	5.45	125.39	113.40
1	A	163	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	23	GLY	CA-C-N	-5.43	105.26	117.20
1	A	253	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	99	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	80	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	5	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	A	61	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	A	67	THR	N-CA-CB	-5.22	100.39	110.30
1	A	69	ILE	N-CA-CB	-5.13	98.99	110.80
1	A	134	ASN	CB-CG-ND2	5.08	128.89	116.70

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	2150	0	2082	25	0
2	A	5	0	0	0	0
3	A	11	0	0	2	0
All	All	2166	0	2082	25	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 (25) 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:145:PRO:O	1:A:166:ARG:HD3	1.96	0.66
1:A:20:ASP:HB2	1:A:24:THR:O	2.05	0.57
1:A:177:ASN:HB3	3:A:275:HOH:O	2.07	0.54
1:A:212:HIS:O	1:A:216:THR:HG23	2.08	0.53
1:A:7:LEU:HG	1:A:32:HIS:CE1	2.45	0.51
1:A:231:ILE:HG23	1:A:248:GLU:HB2	1.93	0.50
1:A:147:HIS:HB2	1:A:163:LEU:HD21	1.95	0.49
1:A:116:LEU:O	1:A:120:LYS:HG2	2.14	0.47
1:A:225:ARG:HG3	1:A:226:PRO:HD2	1.97	0.46
1:A:190:GLN:HE22	1:A:232:ILE:HG21	1.81	0.46
1:A:46:THR:HB	1:A:225:ARG:HB3	1.99	0.45
1:A:112:ILE:HD11	1:A:240:PHE:CE1	2.52	0.45
1:A:39:GLN:NE2	1:A:158:LYS:NZ	2.64	0.45
1:A:93:VAL:O	1:A:96:LYS:HB3	2.17	0.44
1:A:112:ILE:HD11	1:A:240:PHE:HE1	1.82	0.44
1:A:53:ARG:NH1	1:A:75:ASN:O	2.52	0.43
1:A:69:ILE:HD13	1:A:69:ILE:HG21	1.75	0.43
1:A:61:TRP:CD1	1:A:66:ASP:HB3	2.53	0.43
1:A:212:HIS:HE1	1:A:261:PRO:O	2.01	0.42
1:A:147:HIS:CD2	1:A:181:TYR:OH	2.73	0.42
1:A:177:ASN:HB3	3:A:266:HOH:O	2.19	0.42
1:A:215:GLN:HE21	1:A:215:GLN:H	1.68	0.42
1:A:182:ALA:O	1:A:186:HIS:HD2	2.03	0.41
1:A:92:PRO:HG2	1:A:141:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HD12	1:A:264:ILE:HA	1.93	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	262/264 (99%)	252 (96%)	10 (4%)	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	233/233 (100%)	201 (86%)	32 (14%)	3	2

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	LEU
1	A	21	ARG
1	A	37	ASN
1	A	39	GLN

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Mol	Chain	Res	Type
1	A	47	THR
1	A	48	LYS
1	A	49	ARG
1	A	50	CYS
1	A	60	LEU
1	A	64	GLN
1	A	66	ASP
1	A	67	THR
1	A	76	ASN
1	A	112	ILE
1	A	120	LYS
1	A	130	VAL
1	A	134	ASN
1	A	138	LEU
1	A	143	LEU
1	A	163	LEU
1	A	166	ARG
1	A	184	LEU
1	A	195	GLU
1	A	215	GLN
1	A	218	LEU
1	A	220	LEU
1	A	225	ARG
1	A	231	ILE
1	A	238	SER
1	A	241	ASP
1	A	249	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	33	GLN
1	A	39	GLN
1	A	73	HIS
1	A	134	ASN
1	A	147	HIS
1	A	162	GLN
1	A	186	HIS
1	A	190	GLN
1	A	212	HIS

### 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 ⓘ

1 ligand is 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	265	-	4,4,4	1.86	1 (25%)	6,6,6	1.75	3 (50%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	265	PO4	P-O1	3.40	1.58	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	265	PO4	O4-P-O3	2.59	116.27	107.97
2	A	265	PO4	O3-P-O1	-2.44	101.98	110.89
2	A	265	PO4	O3-P-O2	2.01	114.43	107.97

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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.