Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2024 – 06:21 PM EST

PDB ID	:	4TMS
Title	:	PLASTIC ADAPTATION TOWARD MUTATIONS IN PROTEINS: STRUCTURAL COMPARISON OF THYMIDYLATE SYNTHASES
Authors	:	Finer-Moore, J.; Stroud, R.
Deposited on	:	1992-01-07
Resolution	:	2.35 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
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:

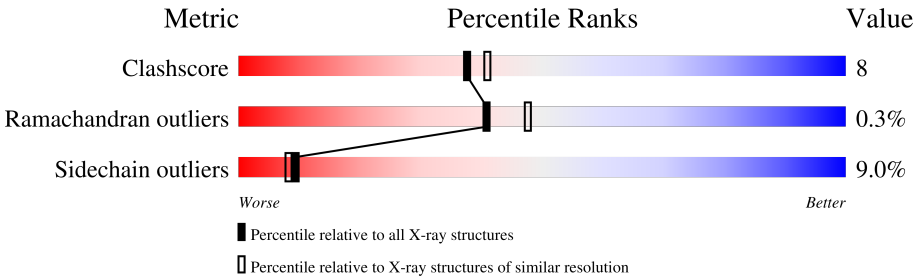
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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 of 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	A	316	68% 26% 6% •

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	317	-	X	-	-

2 Entry composition

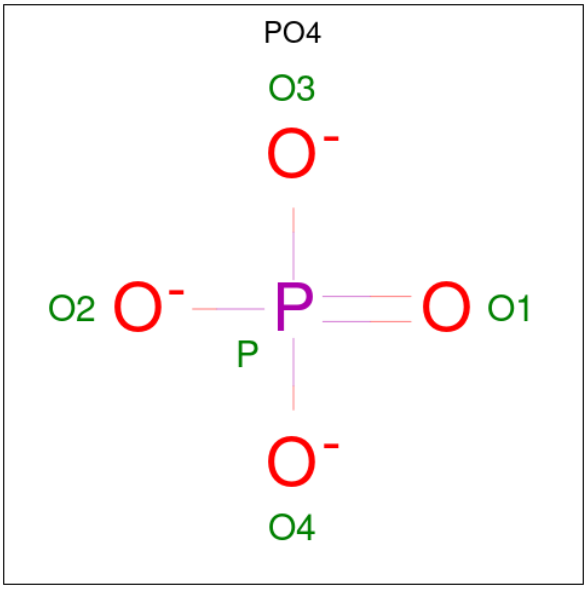
There are 3 unique types of molecules in this entry. The entry contains 2634 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	316	2590	1677	438	467	8	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	39	39	39	0	0

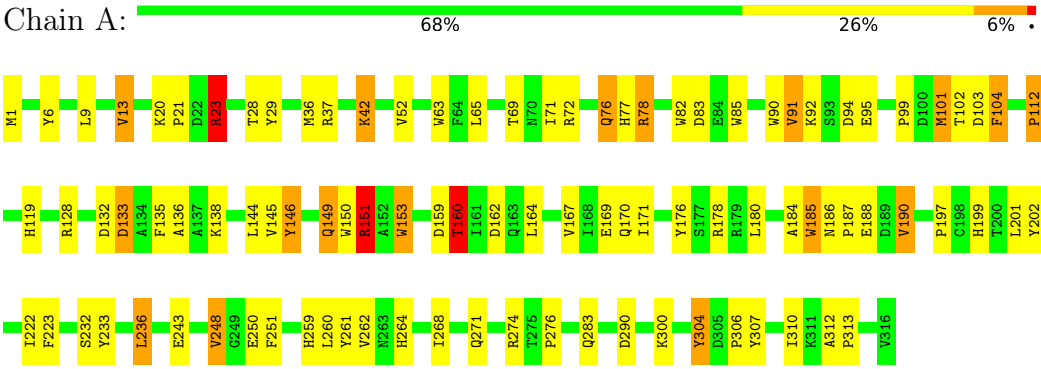
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	78.30Å 78.30Å 243.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2634	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.03	3/2674 (0.1%)	1.84	63/3634 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ARG	CG-CD	-6.64	1.35	1.51
1	A	82	TRP	CG-CD2	-5.36	1.34	1.43
1	A	250	GLU	CD-OE2	-5.10	1.20	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	ARG	NH1-CZ-NH2	-15.10	102.79	119.40
1	A	178	ARG	NE-CZ-NH2	14.29	127.44	120.30
1	A	23	ARG	NE-CZ-NH1	-13.94	113.33	120.30
1	A	37	ARG	NE-CZ-NH2	13.04	126.82	120.30
1	A	233	TYR	CB-CG-CD1	-11.06	114.36	121.00
1	A	23	ARG	NE-CZ-NH2	10.54	125.57	120.30
1	A	150	TRP	CD1-CG-CD2	9.98	114.29	106.30
1	A	178	ARG	NE-CZ-NH1	-9.81	115.39	120.30
1	A	85	TRP	CD1-CG-CD2	8.77	113.32	106.30
1	A	63	TRP	CD1-CG-CD2	8.36	112.99	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	A	90	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	A	153	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	A	85	TRP	CE2-CD2-CG	-7.87	101.00	107.30
1	A	201	LEU	CA-CB-CG	7.70	133.00	115.30
1	A	307	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	A	185	TRP	CD1-CG-CD2	7.37	112.20	106.30
1	A	78	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	A	150	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	A	82	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	150	TRP	CG-CD1-NE1	-7.26	102.84	110.10
1	A	90	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A	176	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	A	37	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	153	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	A	52	VAL	CG1-CB-CG2	-6.78	100.05	110.90
1	A	160	THR	N-CA-CB	-6.73	97.52	110.30
1	A	6	TYR	CB-CG-CD2	-6.68	117.00	121.00
1	A	103	ASP	CA-C-N	-6.55	102.78	117.20
1	A	190	VAL	CA-CB-CG2	-6.51	101.14	110.90
1	A	185	TRP	CE2-CD2-CG	-6.35	102.22	107.30
1	A	167	VAL	CG1-CB-CG2	-6.32	100.79	110.90
1	A	77	HIS	CA-CB-CG	-6.25	102.97	113.60
1	A	85	TRP	CG-CD2-CE3	6.24	139.51	133.90
1	A	82	TRP	CE2-CD2-CG	-6.22	102.32	107.30
1	A	1	MET	CG-SD-CE	6.18	110.09	100.20
1	A	63	TRP	CE2-CD2-CG	-6.17	102.36	107.30
1	A	91	VAL	CA-CB-CG2	-6.13	101.71	110.90
1	A	304	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	63	TRP	CG-CD1-NE1	-5.97	104.13	110.10
1	A	36	MET	CG-SD-CE	5.96	109.73	100.20
1	A	151	ARG	CA-CB-CG	-5.88	100.46	113.40
1	A	146	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	261	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	A	176	TYR	CG-CD2-CE2	-5.57	116.84	121.30
1	A	90	TRP	CB-CG-CD1	-5.54	119.79	127.00
1	A	42	LYS	CA-C-N	5.41	127.03	116.20
1	A	85	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	A	274	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	63	TRP	CG-CD2-CE3	5.33	138.69	133.90
1	A	78	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	202	TYR	CA-CB-CG	5.29	123.44	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	A	169	GLU	CA-CB-CG	5.27	124.99	113.40
1	A	132	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	13	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	A	83	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	159	ASP	CA-CB-CG	5.15	124.73	113.40
1	A	90	TRP	CG-CD2-CE3	5.13	138.52	133.90
1	A	251	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	236	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	248	VAL	N-CA-CB	-5.08	100.32	111.50
1	A	232	SER	N-CA-CB	5.02	118.03	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain

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	2590	0	2496	39	0
2	A	5	0	0	1	0
3	A	39	0	0	1	0
All	All	2634	0	2496	39	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 8.

All (39) 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:260:LEU:HD21	1:A:268:ILE:HG21	1.80	0.64
1:A:69:THR:HG22	1:A:145:VAL:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:HG2	1:A:162:ASP:OD2	2.04	0.57
1:A:13:VAL:HG21	1:A:222:ILE:CD1	2.36	0.56
1:A:184:ALA:O	1:A:197:PRO:HG2	2.05	0.56
1:A:185:TRP:CZ2	1:A:190:VAL:HG11	2.41	0.56
1:A:283:GLN:HB3	1:A:300:LYS:HB2	1.88	0.54
1:A:112:PRO:HG2	1:A:114:PHE:HB3	1.91	0.52
1:A:223:PHE:CE1	1:A:312:ALA:HB2	2.45	0.50
1:A:171:ILE:HG12	1:A:180:LEU:HD13	1.93	0.49
1:A:72:ARG:HG2	1:A:76:GLN:NE2	2.27	0.48
1:A:69:THR:HG22	1:A:145:VAL:CG1	2.44	0.48
1:A:112:PRO:HG2	1:A:114:PHE:CB	2.44	0.48
1:A:102:THR:HA	3:A:340:HOH:O	2.14	0.47
1:A:72:ARG:HH12	1:A:133:ASP:HA	1.79	0.47
1:A:91:VAL:HG11	1:A:104:PHE:HE1	1.80	0.47
1:A:271:GLN:HB2	1:A:310:ILE:CD1	2.44	0.47
1:A:223:PHE:HE1	1:A:312:ALA:HB2	1.79	0.47
1:A:72:ARG:HG2	1:A:76:GLN:HE22	1.80	0.46
1:A:99:PRO:HB2	1:A:101:MET:HE1	1.98	0.46
1:A:153:TRP:O	1:A:160:THR:HA	2.15	0.46
1:A:264:HIS:NE2	1:A:313:PRO:O	2.45	0.46
1:A:13:VAL:HG21	1:A:222:ILE:HD11	1.99	0.45
1:A:71:ILE:HD13	1:A:71:ILE:HA	1.71	0.44
1:A:20:LYS:HA	1:A:21:PRO:HD2	1.72	0.43
1:A:29:TYR:HE2	1:A:262:VAL:HG22	1.82	0.43
1:A:128:ARG:HB3	1:A:135:PHE:CD2	2.54	0.43
1:A:72:ARG:HH11	1:A:136:ALA:HB2	1.84	0.43
1:A:23:ARG:NH1	2:A:317:PO4:O2	2.52	0.42
1:A:149:GLN:HE21	1:A:149:GLN:HB3	1.71	0.42
1:A:116:ALA:HA	1:A:119:HIS:HB2	2.01	0.42
1:A:115:ALA:O	1:A:119:HIS:CD2	2.74	0.41
1:A:264:HIS:CD2	1:A:312:ALA:HB1	2.55	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.94	0.41
1:A:186:ASN:HA	1:A:187:PRO:HD3	1.91	0.41
1:A:199:HIS:HB3	1:A:215:LEU:HD21	2.03	0.41
1:A:146:TYR:HA	1:A:149:GLN:HG2	2.03	0.40
1:A:28:THR:HB	1:A:259:HIS:HB2	2.03	0.40
1:A:304:TYR:CZ	1:A:306:PRO:HB3	2.57	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	314/316 (99%)	293 (93%)	20 (6%)	1 (0%)	41 47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	PRO

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	277/278 (100%)	252 (91%)	25 (9%)	9 8

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	23	ARG
1	A	42	LYS
1	A	65	LEU
1	A	76	GLN
1	A	78	ARG
1	A	92	LYS
1	A	94	ASP
1	A	95	GLU
1	A	101	MET

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Mol	Chain	Res	Type
1	A	104	PHE
1	A	133	ASP
1	A	138	LYS
1	A	149	GLN
1	A	151	ARG
1	A	160	THR
1	A	164	LEU
1	A	170	GLN
1	A	188	GLU
1	A	215	LEU
1	A	236	LEU
1	A	243	GLU
1	A	248	VAL
1	A	276	PRO
1	A	290	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	119	HIS
1	A	149	GLN
1	A	207	ASN

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 monosaccharides 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	317	-	4,4,4	2.43	3 (75%)	6,6,6	2.26	3 (50%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	PO4	P-O1	2.95	1.57	1.50
2	A	317	PO4	P-O2	-2.66	1.46	1.54
2	A	317	PO4	P-O3	-2.11	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	317	PO4	O4-P-O2	3.44	119.00	107.97
2	A	317	PO4	O2-P-O1	-2.63	101.28	110.89
2	A	317	PO4	O4-P-O1	-2.13	103.08	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	317	PO4	1	0

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

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.