



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:35 PM EDT

PDB ID : 3MBM / pdb_00003mbm
Title : Crystal structure of 2C-methyl-D-erythritol 2,4-cyclodiphosphate synthase from Burkholderia pseudomallei with cytosine and FoL fragment 717, imidazole[2,1-b][1,3]thiazol-6-ylmethanol
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2010-03-25
Resolution : 1.80 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 1.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

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
4	717	C	163	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3743 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 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	1	0
			1183	742	220	218	3			
1	B	154	Total	C	N	O	S	0	1	0
			1132	711	207	211	3			
1	C	151	Total	C	N	O	S	0	1	0
			1114	701	204	206	3			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q63T71
A	-19	ALA	-	expression tag	UNP Q63T71
A	-18	HIS	-	expression tag	UNP Q63T71
A	-17	HIS	-	expression tag	UNP Q63T71
A	-16	HIS	-	expression tag	UNP Q63T71
A	-15	HIS	-	expression tag	UNP Q63T71
A	-14	HIS	-	expression tag	UNP Q63T71
A	-13	HIS	-	expression tag	UNP Q63T71
A	-12	MET	-	expression tag	UNP Q63T71
A	-11	GLY	-	expression tag	UNP Q63T71
A	-10	THR	-	expression tag	UNP Q63T71
A	-9	LEU	-	expression tag	UNP Q63T71
A	-8	GLU	-	expression tag	UNP Q63T71
A	-7	ALA	-	expression tag	UNP Q63T71
A	-6	GLN	-	expression tag	UNP Q63T71
A	-5	THR	-	expression tag	UNP Q63T71
A	-4	GLN	-	expression tag	UNP Q63T71
A	-3	GLY	-	expression tag	UNP Q63T71
A	-2	PRO	-	expression tag	UNP Q63T71
A	-1	GLY	-	expression tag	UNP Q63T71
A	0	SER	-	expression tag	UNP Q63T71
B	-20	MET	-	expression tag	UNP Q63T71
B	-19	ALA	-	expression tag	UNP Q63T71

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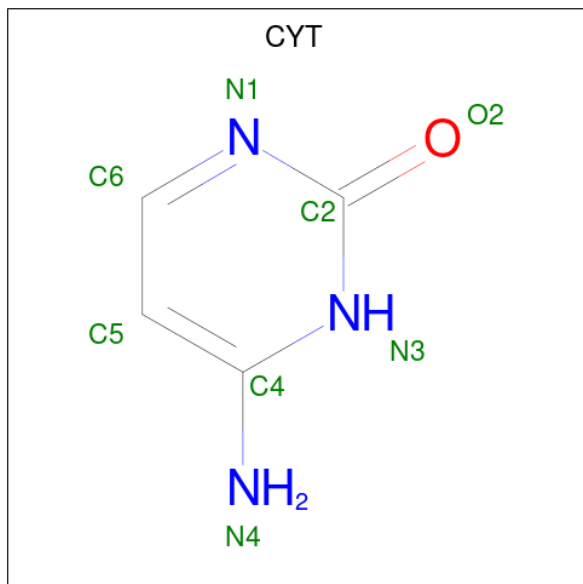
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP Q63T71
B	-17	HIS	-	expression tag	UNP Q63T71
B	-16	HIS	-	expression tag	UNP Q63T71
B	-15	HIS	-	expression tag	UNP Q63T71
B	-14	HIS	-	expression tag	UNP Q63T71
B	-13	HIS	-	expression tag	UNP Q63T71
B	-12	MET	-	expression tag	UNP Q63T71
B	-11	GLY	-	expression tag	UNP Q63T71
B	-10	THR	-	expression tag	UNP Q63T71
B	-9	LEU	-	expression tag	UNP Q63T71
B	-8	GLU	-	expression tag	UNP Q63T71
B	-7	ALA	-	expression tag	UNP Q63T71
B	-6	GLN	-	expression tag	UNP Q63T71
B	-5	THR	-	expression tag	UNP Q63T71
B	-4	GLN	-	expression tag	UNP Q63T71
B	-3	GLY	-	expression tag	UNP Q63T71
B	-2	PRO	-	expression tag	UNP Q63T71
B	-1	GLY	-	expression tag	UNP Q63T71
B	0	SER	-	expression tag	UNP Q63T71
C	-20	MET	-	expression tag	UNP Q63T71
C	-19	ALA	-	expression tag	UNP Q63T71
C	-18	HIS	-	expression tag	UNP Q63T71
C	-17	HIS	-	expression tag	UNP Q63T71
C	-16	HIS	-	expression tag	UNP Q63T71
C	-15	HIS	-	expression tag	UNP Q63T71
C	-14	HIS	-	expression tag	UNP Q63T71
C	-13	HIS	-	expression tag	UNP Q63T71
C	-12	MET	-	expression tag	UNP Q63T71
C	-11	GLY	-	expression tag	UNP Q63T71
C	-10	THR	-	expression tag	UNP Q63T71
C	-9	LEU	-	expression tag	UNP Q63T71
C	-8	GLU	-	expression tag	UNP Q63T71
C	-7	ALA	-	expression tag	UNP Q63T71
C	-6	GLN	-	expression tag	UNP Q63T71
C	-5	THR	-	expression tag	UNP Q63T71
C	-4	GLN	-	expression tag	UNP Q63T71
C	-3	GLY	-	expression tag	UNP Q63T71
C	-2	PRO	-	expression tag	UNP Q63T71
C	-1	GLY	-	expression tag	UNP Q63T71
C	0	SER	-	expression tag	UNP Q63T71

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

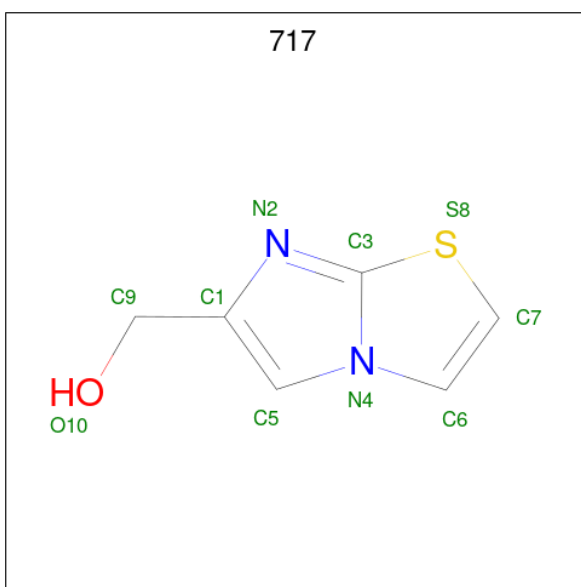
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 6-AMINOPYRIMIDIN-2(1H)-ONE (CCD ID: CYT) (formula: $C_4H_5N_3O$).



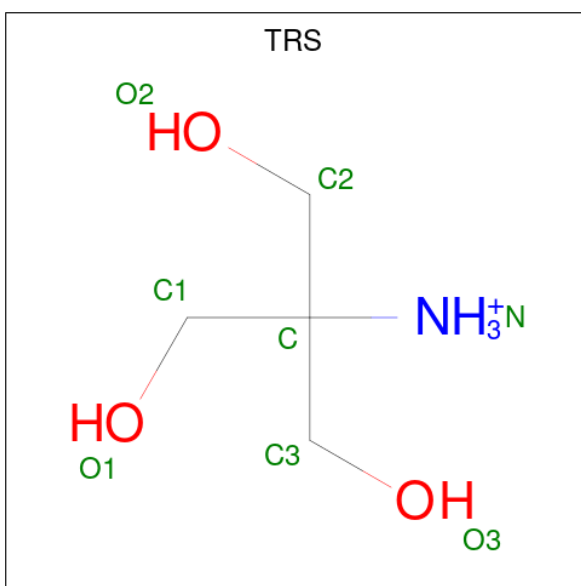
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	3	1		
3	B	1	Total	C	N	O	0	0
			8	4	3	1		
3	C	1	Total	C	N	O	0	0
			8	4	3	1		

- Molecule 4 is imidazo[2,1-b][1,3]thiazol-6-ylmethanol (CCD ID: 717) (formula: $C_6H_6N_2OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			10	6	2	1	1		
4	B	1	Total	C	N	O	S	0	0
			10	6	2	1	1		
4	C	1	Total	C	N	O	S	0	0
			10	6	2	1	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			16	8	2	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		
6	B	45	Total	O	0	0
			45	45		
6	C	63	Total	O	0	0
			63	63		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.54Å 67.57Å 60.03Å 90.00° 96.12° 90.00°	Depositor
Resolution (Å)	25.50 – 1.80	Depositor
% Data completeness (in resolution range)	96.0 (25.50-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.217	Depositor
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.157	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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
4	717	A	165	2	11,11,11	2.11	5 (45%)	13,15,15	1.73	3 (23%)
5	TRS	A	166[A]	-	7,7,7	0.20	0	9,9,9	0.55	0
4	717	B	165	2	11,11,11	2.31	6 (54%)	13,15,15	1.56	3 (23%)
4	717	C	163	2	11,11,11	2.44	5 (45%)	13,15,15	2.32	7 (53%)
3	CYT	B	164	-	7,8,8	1.37	1 (14%)	7,10,10	2.52	3 (42%)
5	TRS	A	166[B]	-	7,7,7	0.37	0	9,9,9	0.62	0
3	CYT	C	165	-	7,8,8	1.97	3 (42%)	7,10,10	3.40	3 (42%)
3	CYT	A	164	-	7,8,8	1.97	3 (42%)	7,10,10	2.88	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	717	A	165	2	-	2/2/2/2	0/2/2/2
5	TRS	A	166[A]	-	-	6/9/9/9	-
4	717	B	165	2	-	2/2/2/2	0/2/2/2
4	717	C	163	2	-	2/2/2/2	0/2/2/2
3	CYT	B	164	-	-	-	0/1/1/1
5	TRS	A	166[B]	-	-	3/9/9/9	-
3	CYT	C	165	-	-	-	0/1/1/1
3	CYT	A	164	-	-	-	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	163	717	C3-N2	4.75	1.41	1.31
4	C	163	717	C3-N4	-3.85	1.34	1.39
3	A	164	CYT	C4-N3	-3.65	1.32	1.37
4	B	165	717	C3-N2	3.48	1.39	1.31
3	C	165	CYT	C4-N3	-3.44	1.32	1.37
4	B	165	717	C6-C7	3.37	1.40	1.33
4	B	165	717	C5-C1	3.29	1.41	1.36
4	B	165	717	C3-N4	-3.23	1.35	1.39
4	C	163	717	C6-C7	3.13	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	165	717	C3-N4	-3.11	1.35	1.39
4	A	165	717	C5-C1	3.07	1.41	1.36
4	A	165	717	C3-S8	-3.05	1.68	1.74
4	C	163	717	C5-C1	3.02	1.41	1.36
4	A	165	717	C6-C7	2.82	1.39	1.33
4	B	165	717	C3-S8	-2.72	1.68	1.74
3	A	164	CYT	C5-C4	2.70	1.43	1.39
4	A	165	717	C3-N2	2.66	1.37	1.31
4	C	163	717	C3-S8	-2.60	1.69	1.74
3	C	165	CYT	C5-C4	2.58	1.43	1.39
3	C	165	CYT	C5-C6	-2.34	1.34	1.39
3	A	164	CYT	C5-C6	-2.15	1.34	1.39
3	B	164	CYT	C5-C4	2.09	1.42	1.39
4	B	165	717	C9-C1	2.03	1.51	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	165	CYT	C5-C4-N3	6.59	121.80	118.04
3	A	164	CYT	C5-C4-N3	5.60	121.23	118.04
3	C	165	CYT	C5-C6-N1	-4.85	120.91	124.75
4	C	163	717	C9-C1-C5	-4.25	122.78	130.38
3	B	164	CYT	C5-C4-N3	4.20	120.43	118.04
3	A	164	CYT	C5-C6-N1	-4.08	121.52	124.75
3	B	164	CYT	C5-C6-N1	-3.56	121.93	124.75
3	C	165	CYT	C5-C4-N4	-3.46	120.52	123.88
4	A	165	717	C9-C1-C5	-3.43	124.25	130.38
4	C	163	717	C7-S8-C3	3.40	93.71	89.76
4	C	163	717	C3-N2-C1	-3.18	100.60	104.97
4	A	165	717	C7-C6-N4	-3.15	109.06	112.27
4	B	165	717	C7-C6-N4	-3.11	109.09	112.27
3	B	164	CYT	C5-C4-N4	-3.04	120.92	123.88
3	A	164	CYT	C5-C4-N4	-2.93	121.03	123.88
4	B	165	717	C9-C1-C5	-2.84	125.31	130.38
4	C	163	717	C7-C6-N4	-2.54	109.68	112.27
4	A	165	717	C9-C1-N2	2.53	125.86	119.34
4	C	163	717	C6-N4-C3	2.35	118.51	113.22
4	C	163	717	C9-C1-N2	2.25	125.14	119.34
4	B	165	717	C9-C1-N2	2.06	124.65	119.34
4	C	163	717	S8-C3-N4	-2.06	108.87	110.51

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	166[A]	TRS	C1-C-C3-O3
5	A	166[A]	TRS	C2-C-C3-O3
5	A	166[A]	TRS	N-C-C3-O3
5	A	166[B]	TRS	C1-C-C3-O3
5	A	166[B]	TRS	C2-C-C3-O3
5	A	166[B]	TRS	N-C-C3-O3
4	B	165	717	N2-C1-C9-O10
5	A	166[A]	TRS	C3-C-C1-O1
4	A	165	717	N2-C1-C9-O10
4	C	163	717	N2-C1-C9-O10
4	A	165	717	C5-C1-C9-O10
4	B	165	717	C5-C1-C9-O10
4	C	163	717	C5-C1-C9-O10
5	A	166[A]	TRS	C2-C-C1-O1
5	A	166[A]	TRS	N-C-C1-O1

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.