

Table S1. A comprehensive summary of all adenosine kinase structures published as of 2010, including the TbrAK structures presented in this work.

PDB code	species	ligand	lid domain conformation
3OTX	<i>T. b. rhodesiense</i>	diadenosine pentaphosphate (AP5A)	closed
2XTB	<i>T. b. rhodesiense</i>	4-[5-(4-phenoxyphenyl)-2H-pyrazol-3-yl]-morpholine (compound 1)	open
1BX4 [1]	<i>H. sapiens</i>	two adenosines	closed
2I6A [2]	<i>H. sapiens</i>	5-iodo-5'-deoxytubercidin	closed
2I6B [2]	<i>H. sapiens</i>	alkynylpyrimidine compound: 5-[4-(dimethylamino)phenyl]-6-[6-morpholin-4-ylpyridin-3-ylethynyl]pyrimidin-4-ylamine	open
1DGM [3]	<i>T. gondii</i>	adenosine	open
1LIO [4]	<i>T. gondii</i>	apo	open
1LIK [4]	<i>T. gondii</i>	two adenosines	closed
1LII [4]	<i>T. gondii</i>	adenosine, β,γ -methylene-adenosine 5'-triphosphate (AMP-PCP, a nonhydrolysable ATP analog)	closed
1LIJ [4]	<i>T. gondii</i>	7-iodotubercidin, β,γ -methylene-adenosine 5'-triphosphate (AMP-PCP, a nonhydrolysable ATP analog)	closed
2ABS [5]	<i>T. gondii</i>	β,γ -methylene-adenosine 5'-triphosphate (AMP-PCP, a nonhydrolysable ATP analog) in two different conformations still undefined density in the adenosine binding site, 6-[(4-nitrobenzyl)thio]-9- β -D-ribofuranosylpurine was added in the crystallization setup	semi-closed
2A9Y [6]	<i>T. gondii</i>	two N ⁶ ,N ⁶ -dimethyladenosine	semi-closed
2A9Z [6]	<i>T. gondii</i>	N ⁶ ,N ⁶ -dimethyladenosine, β,γ -methylene-adenosine 5'-triphosphate (AMP-PCP, a nonhydrolysable ATP analog)	semi-closed
2AA0 [6]	<i>T. gondii</i>	two 6-methyl mercaptopurine riboside	semi-closed
2AB8 [6]	<i>T. gondii</i>	6-methyl mercaptopurine riboside, β,γ -methylene-adenosine 5'-triphosphate (AMP-PCP, a nonhydrolysable ATP analog)	semi-closed
2PKF [7]	<i>M. tuberculosis</i>	apo	open
2PKM [7]	<i>M. tuberculosis</i>	adenosine	closed
2PKK [7]	<i>M. tuberculosis</i>	2-fluoroadenosine	closed
2PKN [7]	<i>M. tuberculosis</i>	β,γ -methylene-adenosine 5'-triphosphate (AMP-PCP, a nonhydrolysable ATP analog)	open

References

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