

Supplementary Table S3 to the manuscript “Common mechanism of activated catalysis in P-loop fold nucleoside triphosphatases – united in diversity”

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The pKa values of Asp256 WB of the bovine ATP synthase as calculated for different states of the catalytic pocket by application of the PROPKA v. 2.0 software [1]

PDB ID, res.	ADP:AlF ₄ ⁻	ADP:AlF ₃	ADP:BeF ₃	ANP	ATP	ADP+P _i	ADP	P _i	Empty	Ref
1E1R, 2.5 Å								1.82		[2]
1E1R, 2.5 Å				9.64						[2]
1e1R, 2.5 Å		9.46								[2]
1E1Q, 2.6 Å							9.03			[2]
1E1Q, 2.6 Å								2.39		[2]
1E1Q, 2.6 Å				8.92						[2]
1H8E, 2.0 Å	8.98									[3]
1H8E, 2.0 Å						5.41				[3]
1H8E, 2.0 Å	8.83									[3]
1W0J, 2.2 Å			9.43							[4]
1W0J, 2.2 Å								2.17		[4]
1W0J, 2.2 Å			9.11							[4]
1H8H, 2.9 Å							9.10			[5]
1H8H, 2.9 Å								2.33		[5]
1H8H, 2.9 Å					8.76					[5]
2CK3, 1.9 Å							9.25			[6]
2CK3, 1.9 Å				9.20						[6]
2CK3, 1.9 Å								2.93		[6]
2JDI, 1.9 Å				9.39						[7]
2JDI, 1.9 Å									2.97	[7]
2JDI, 1.9 Å				9.32						[7]
2JIZ, 2.3 Å							9.51			[8]
2JIZ, 2.3 Å								2.07		[8]
2JIZ, 2.3 Å				9.26						[8]

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