Supplementary Table S1. X-ray crystallography data and refinement statistics.

	dUTPase with inhibitor (PDB ID: 5H4J)
Crystal data	
$P2_13$ cell dimensions (Å)	a = 89.64, b = 89.64, c = 89.64
Resolution range (Å)	51.76–1.80 (1.86–1.80)
No. of observed reflections	492525
No. of unique reflections	21554
Completeness of data (%)	99.9 (99.7)
R_{merge} (%)[a]	0.064 (0.237)
Average I/σI	24.9 (10.4)
Refinement statistics	
Resolution range (Å)	40.10–1.80 (1.82–1.80)
R_{work} (%)[b]	17.0 (21.70)
No. of reflections in work set	20338 (1462)
R_{free} (%)[c]	17.3 (24.60)
No. of reflections in test set	1140 (82)
Rmsd bonds (Å)[d]	0.019
Rmsd angles (°)[d]	2.049
No. of nonhydrogen atoms	1163
No. of protein/inhibitor/water/Zn/dimethyl sulfoxide/imidazole atoms	982/31/140/1/4/5
Average B-factor (Å^2) for all atoms	24.99
Average B-factor (Å^2) for protein/inhibitor/water/Zn/dimethyl sulfoxide/imidazole	23.95/20.77/33.21/19.6/35.55/19.7

[a] $R_{merge} = \Sigma_{hkl} \Sigma_i |I_i(hkl) - \langle I(hkl) \rangle| / \Sigma_{hkl} \Sigma_i I_i(hkl)$, where $I_i(hkl)$ is the intensity of an observation, and $\langle I(hkl) \rangle$ is the mean value for its unique reflection; summations are over all reflections.

[b] $R_{work} = \Sigma_{hkl} ||F_o| - |F_c|| / \Sigma_{hkl} |F_o|$, where F_o and F_c are observed and calculated structure factors, respectively.

[c] R_{free} values were calculated for randomly selected 5% of the data that were omitted during refinement.

[d] Root-mean-square deviation from ideal/target geometries.