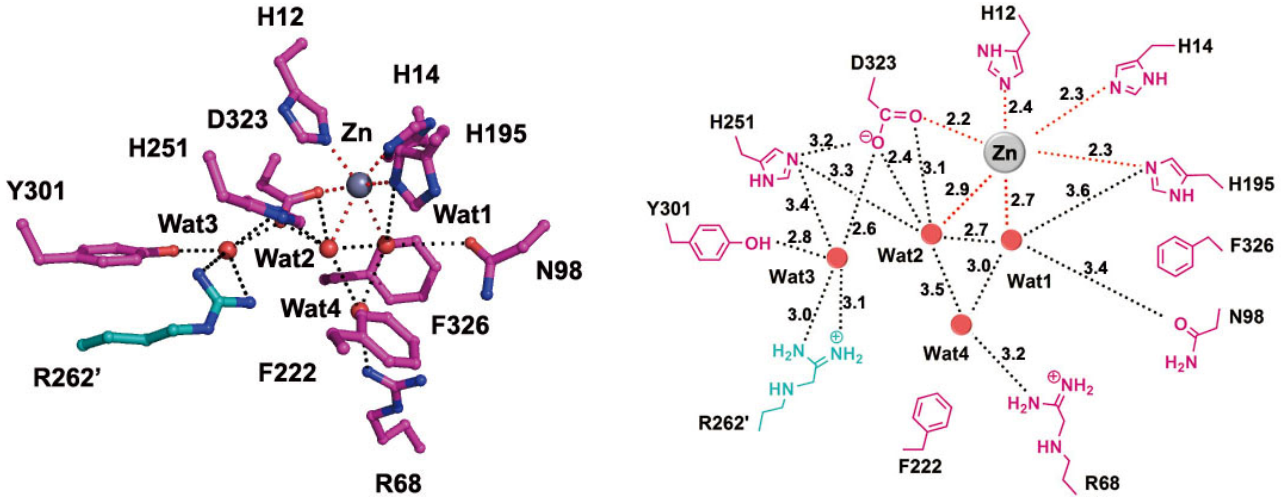
Supplementary information, Figure S6

A



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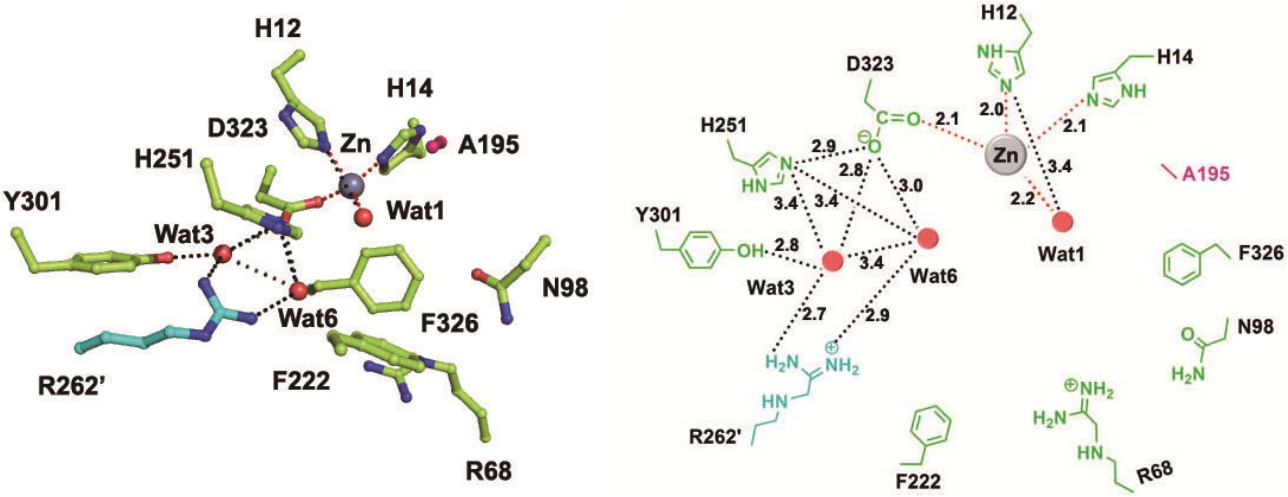
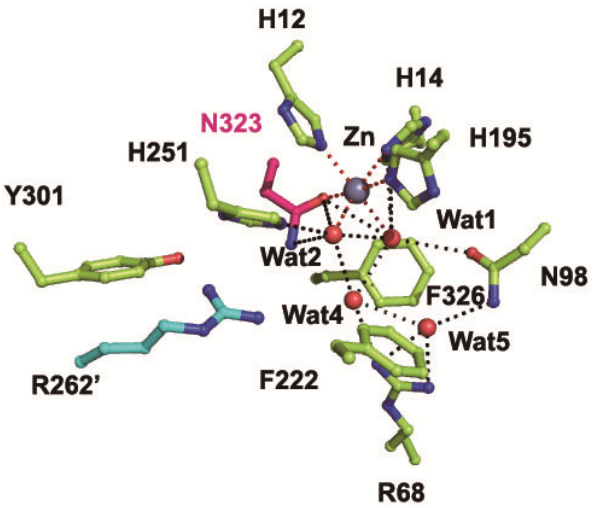


C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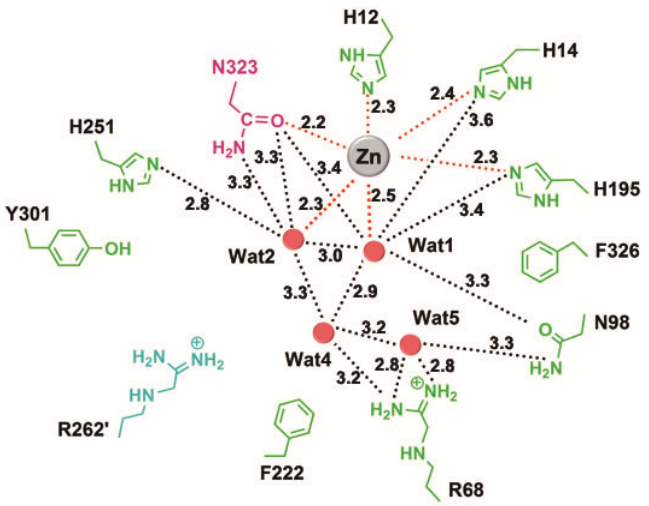
N323
Zn
H195
H251
Y301
Wat1
Wat2
N98
F326
Wat4
Wat5
R262'
F222
R68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H14
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H251
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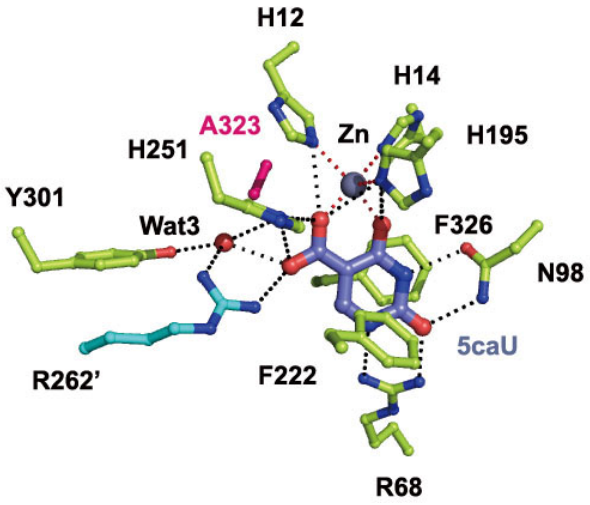
Zn
H195
Wat1
Wat2
F326
N98
Wat5
Wat4
R262'
F222
R68

D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Zn
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H195
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5caU
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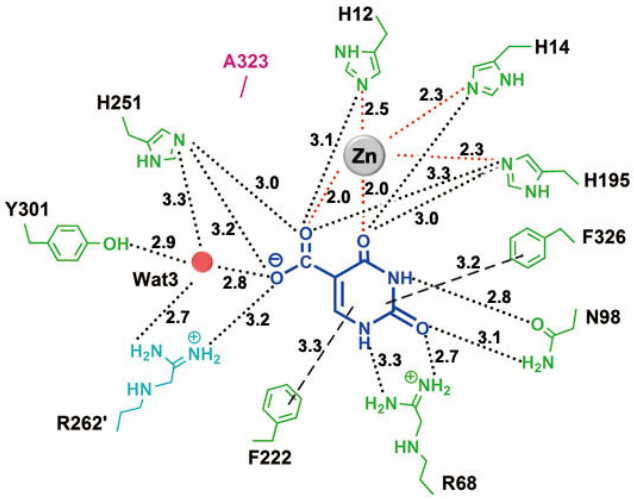
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H14
A323
H251
Zn
H195
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Wat3
F326
N98
R262'
F222
R68

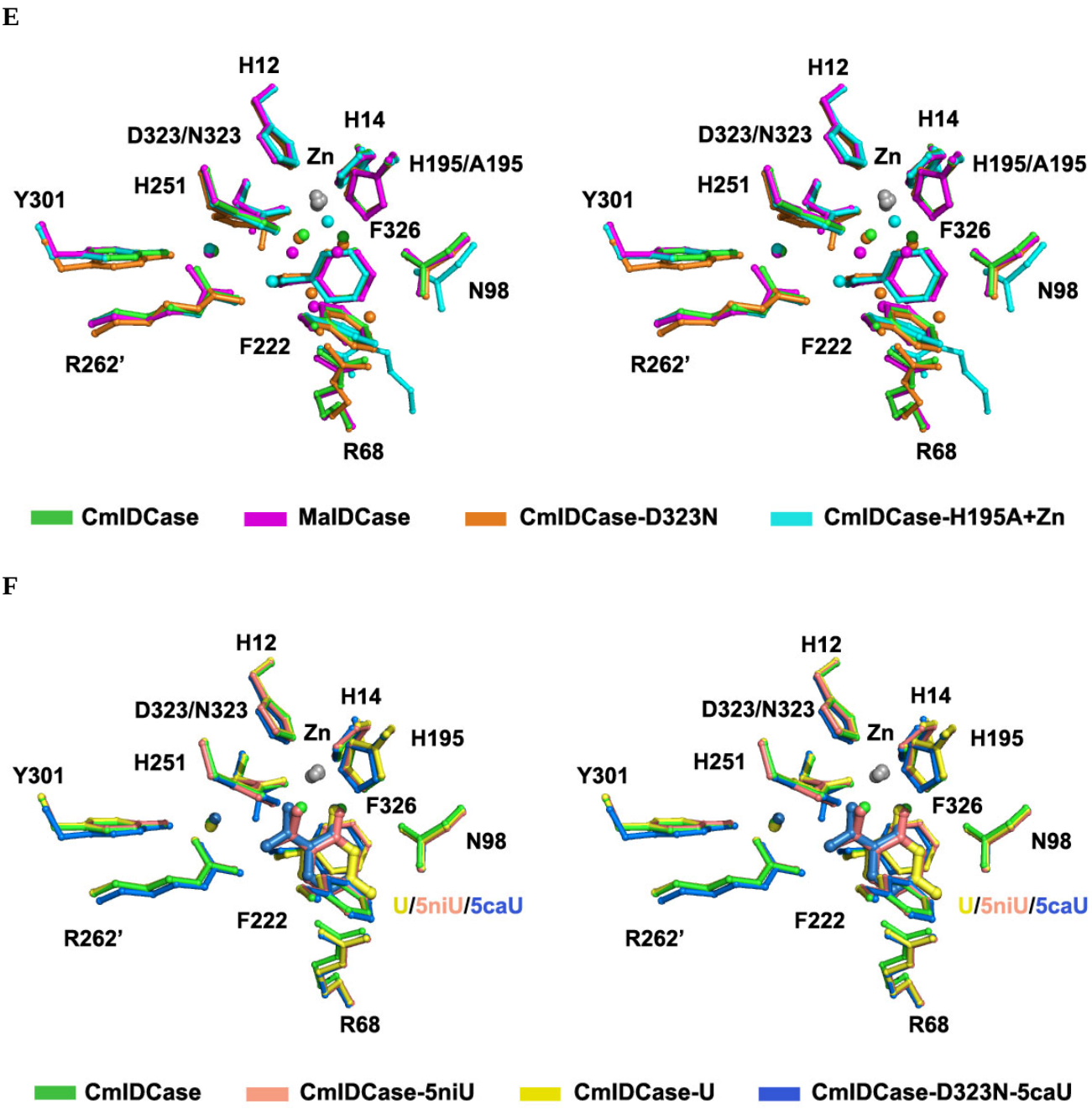

Figure S6 Structure of the active site. Structure of the active site (left panel) and a schematic diagram showing the interactions of the Zn^{2+} and/or the ligand with the surrounding residues (right panel) in **(A)** the apo MaIDCase, **(B)** the apo H195A mutant (cocrystallized with Zn^{2+}), **(C)** the apo D323N mutant, and **(D)** the D323A-5caU complex. The ligands and the key residues involved in the interactions with

the Zn^{2+} and the ligand are shown with ball-and-stick models, the Zn^{2+} with a gray sphere, and the water molecules with red spheres. Arg262 is contributed from an adjacent subunit. The coordination bonds of the Zn^{2+} are indicated with red dotted lines, the hydrogen bonds with black dotted lines, and the key hydrophobic interactions with black dashed lines. All bond lengths (Å) are indicated. **(E)** Comparison of the active site in the structures of the apo CmIDCase (green), the apo MaIDCase (purple), the apo H195A mutant (cyan), and the apo D323A mutant (orange). **(F)** Comparison of the active site in the structures of the apo CmIDCase (green), the CmIDCase-U complex (yellow), the CmIDCase-5niU complex (orange), and the D323N-caU complex (blue).