Supplemental Material

Atomic structures of the RNA end-healing 5'-OH kinase and 2',3'-cyclic phosphodiesterase domains of fungal tRNA ligase: conformational switches in the kinase upon binding of the GTP phosphate donor

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Supplemental Table S1

Supplemental Figures S1, S2, S3, and S4

Table S1: Crystallographic data and refinement statistics

	KIN-CPD	KIN-D445N apo	KIN-D445N•GTP•Mg	KIN-D445N•IDP	KIN-D445N•dGDP	KIN-D445N•GDP•Mg
Data collection						
Beamline	24ID-C	24ID-E	24ID-E	24ID-C	24ID-C	24ID-E
Space group	$P2_1$	$C222_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Cell dimensions a, b, c (Å) α, β, γ (°)	 77.5, 77.7, 79.5 90, 93.5, 90	 55.4, 122.9, 150.6 90, 90, 90	 50.2, 55.7, 81.8 90, 90, 90	 56.7, 58.4, 72.3 90, 90, 90	 50.1, 56.4, 82.5 90, 90, 90	 50.6, 55.4, 81.4 90, 90, 90
Resolution (Å)	50-1.95 (2.0-1.95)	50-1.98 (2.01-1.98)	50-1.85 (1.88-1.85)	50-1.53 (1.56-1.53)	50-1.7 (1.73-1.7)	50-1.71 (1.74-1.71)
Wavelength (Å)	0.9717	0.9791	0.9791	0.9717	0.9717	0.9792
R_{pim}	0.037 (0.356)	0.024 (0.269)	0.036 (0.248)	0.040 (0.301)	0.026 (0.269)	0.035 (0.227)
CC(1/2)	0.998 (0.863)	0.997 (0.842)	1.000 (0.754)	1.000 (0.772)	0.994 (0.803)	0.994 (0.829)
$\langle I \rangle / \langle \sigma I \rangle$	23.0 (2.0)	37.2 (2.2)	29.5 (2.6)	23.0 (2.4)	35.6 (2.4)	32.0 (2.0)
Completeness (%)	96.3 (83.1)	95.8 (73.7)	99.1 (92.3)	97.3 (73.2)	97.4 (77.0)	93.0 (52.0)
Redundancy	3.9 (2.7)	6.1 (5.4)	5.5 (3.9)	3.8 (1.7)	5.8 (4.0)	4.6 (2.7)
Unique reflections	 38436	 34731	 20105	 36059	 25854	 23552
Refinement						
R_{work} / R_{free}	0.185 / 0.221	0.193 / 0.236	0.170 / 0.215	0.174 / 0.208	0.180 / 0.209	0.186 / 0.208
B-factors (Å^2) Average/Wilson	 52.7 / 34.2	 60.1 / 36.5	 33.7/ 24.6	 26.0 / 15.9	 38.6 / 24.3	 32.4 / 23.1
RMS deviations bond lengths (Å) bond angles (°)	 0.007 0.930	 0.009 1.220	 0.007 0.887	 0.006 0.870	 0.006 0.867	 0.006 0.893
Ramachandran % favored % allowed outliers	 96.8 3.2 0	 97.8 2.2 0	 99.0 1.0 0	 99.6 0.4 0	 98.2 1.8 0	 99.0 1.0 0
Model contents						
Protomers/ASU	1	2	1	1	1	1
Protein residues	413	421	216	223	224	211
Ions	1 Mg, 1 PO_4	2 PO_4	1 Mg	1 PO_4	1 PO_4	1 Mg
Ligand	GDP	-	GTP	IDP	dGDP	GDP
Water	168	168	158	259	170	157
PDB ID	6U05	6U00	6U03	6TZX	6TZ0	6TZM

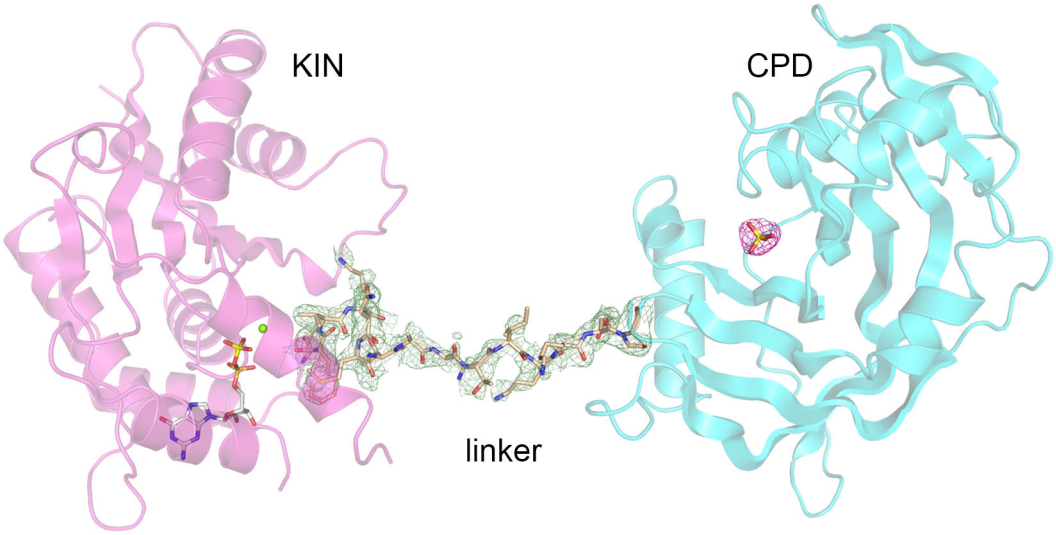

Figure S1. Electron density ($2F_o$-F_c) for the interdomain linker and a phosphate anion in the CPD active site. The KIN-CPD protomer is shown as a cartoon trace. The linker, colored beige, is depicted as a stick model. The density map overlying the linker is shown as a light green mesh contoured at 0.5 σ. The $2F_o$-F_c electron density map overlying the phosphate anion stick model is depicted as a magenta mesh contoured at 1.5 σ.

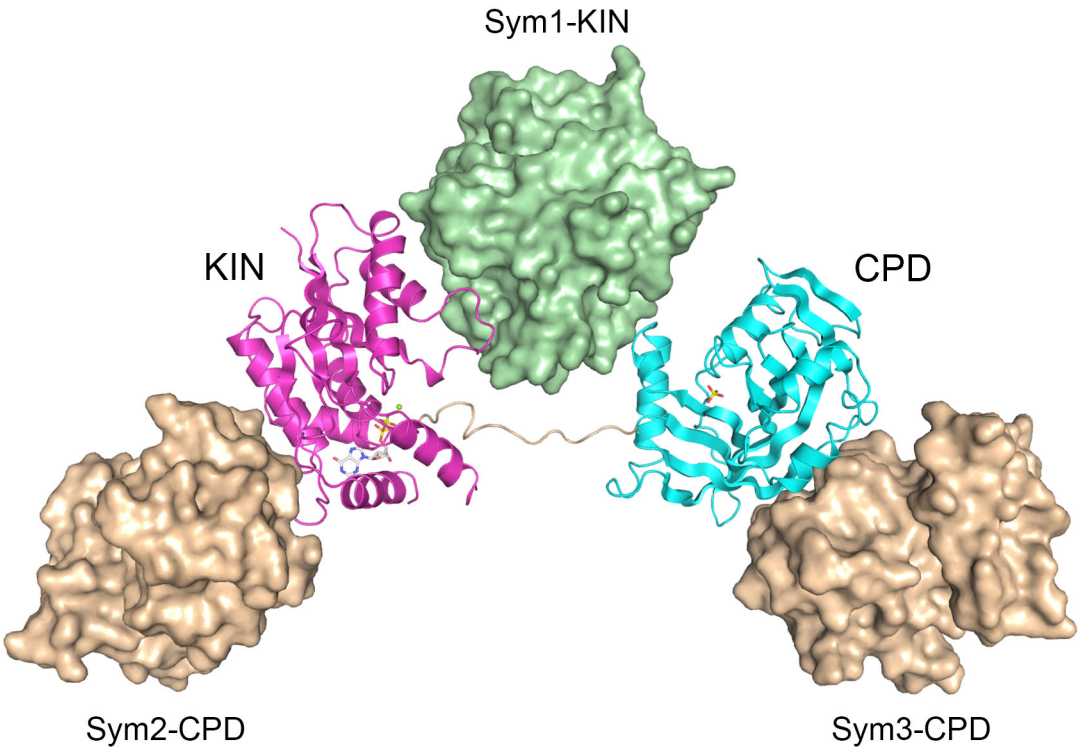

Figure S2. Crystal packing contacts of the KIN-CPD protomer. The KIN-CPD tertiary structure is shown as a cartoon model with the KIN domain in magenta, CPD domain in cyan, and the interdomain linker in beige. Three symmetry related protein molecules (Sym1, Sym2, and Sym3) that abut KIN-CPD in the crystal lattice are shown as surface models. The Sym1 KIN domain (colored light green) packs into the space between the KIN and CPD domains of the protomer and its interface with KIN-CPD comprises an area of 835 $Å^2$. The Sym2 and Sym3 CPD domains (colored beige) pack against the KIN and CPD domains of the protomer, respectively, and their interfaces with the protomer comprise 577 $Å^2$ and 435 $Å^2$, respectively. Analysis of the three interfaces in PISA returned a Complex Formation Significance Score of 0.000, implying that these interfaces are the result of crystal packing only.

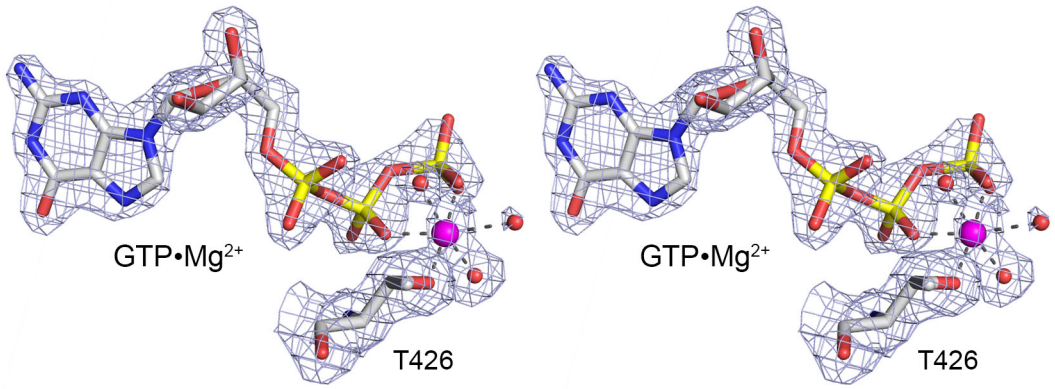

Figure S3. A stereo view of the $2F_o$-F_c simulated annealed omit map contoured at 1.5 σ and superimposed on the refined model of GTP and magnesium in the KIN active site.

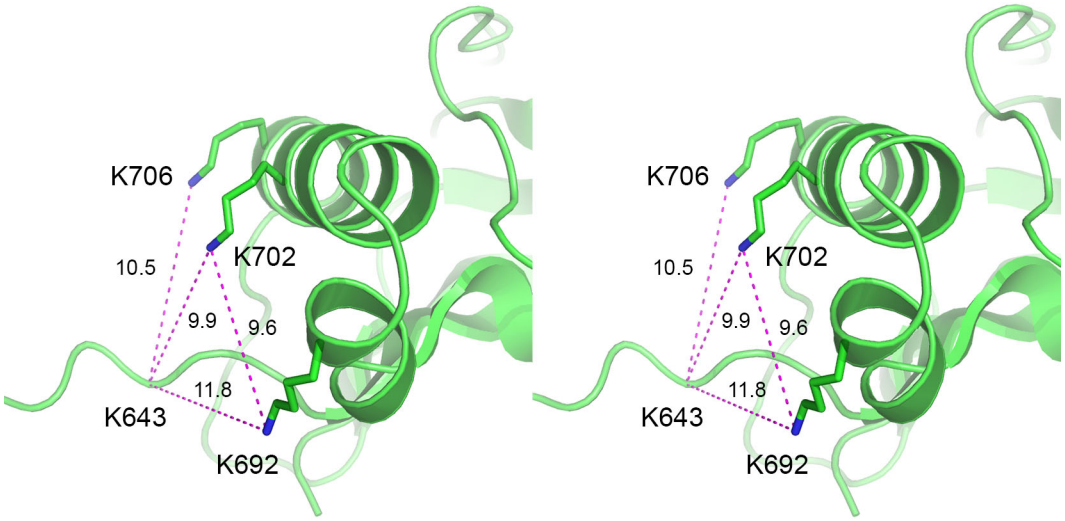

Figure S4. Correlation of lysine chemical crosslinking data for *Coccidioides immitis* CPD with the structure of *Candida albicans* CPD. Stereo depiction of the pairs of lysine crosslinks identified in the CPD domain of *Coccidioides* Trl1 that involve amino acids conserved in *Candida* CPD. The distances (Å) between the K702 and K692 Nζ atoms is shown, as are the distances between the K643 Cα atom (Lys643 being in the linker, we presume that its side chain has no fixed position in solution) and the K692, K702, and K706 Nζ atoms.