Supplemental Data

Structure of 3'-PO_4/5'-OH RNA ligase RtcB in complex with a 5'-OH oligonucleotide

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Table S1. Crystallographic data and refinement statistics

	RtcB•DNA complex
Data collection	
Beamline	APS 24-ID-E
Space group	$P4_32_12$
Cell dimensions a, b, c (Å) α, β, γ (°)	 151.4, 151.4, 82.3 90, 90, 90
Resolution (Å)	50–2.70 (2.75–2.70)
Wavelength (Å)	0.9792
R_{pim}	0.026 (0.411)
CC1/2	0.998 (0.743)
$\langle I \rangle / \langle \sigma I \rangle$	31.7 (2.1)
Completeness (%)	100.0 (100.0)
Redundancy	10.9 (11.1)
Unique reflections	26812
Refinement	
R_{work} / R_{free}	0.191 / 0.216 (0.303 / 0.317)
B-factors (Å^2) Average/Wilson	70.1 / 64.3
RMS deviations bond lengths (Å) bond angles (°)	 0.011 1.351
Ramachandran plot % favored % allowed outliers	 95.4 4.6 0
Model contents	
Protomers / ASU	1
Protein residues	480
Nucleotides	6
Water molecules	17
Ions	2
PDB ID	7LFQ

Values in parentheses refer to the highest resolution shell.

R_{free} set consists of 7.5% reflections chosen randomly against which the structure was not refined.

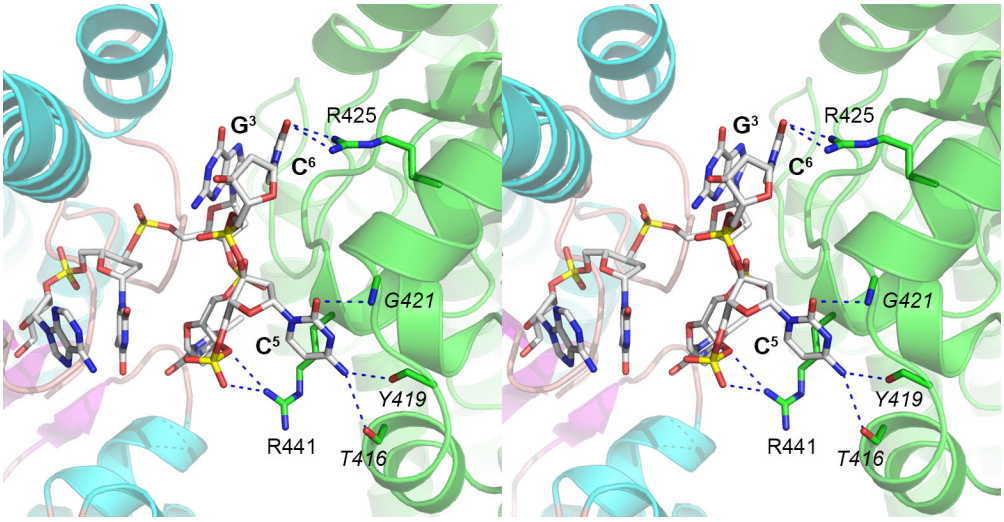

Figure S1. The distal segment of the 5'-OH strand contacts a symmetry-related RtcB protomer. Stereo view of the $_{HO}A^{1}pT^{2}pG^{3}pT^{4}pC^{5}pC^{6}$ strand with its 5'-OH end in the active site of the RtcB protomer at left (cartoon model colored by secondary structure) highlighting an interface of the distal nucleotides with a symmetry-related RtcB protomer in the crystal lattice (green cartoon model). Hydrogen bonds to the oligonucleotide from the symmetry-related RtcB side chains (labeled in plain font) and main chains (labeled in italics) are denoted by blue dashed lines.