Supplemental Information

Structures of RNA ligase RtcB in complexes with divalent cations and GTP

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Supplemental Tables S1 and S2

Table S1. Crystallographic data and refinement statistics.

Structure	PhoRtcB•Mn^{2+}•GTP	PhoRtcB•Co^{2+}•GTP	PhoRtcB•Ni^{2+}•GTP	PhoRtcB•Zn^{2+}•GTP	PhoRtcB•Cu^{2+}•GTP
Data collection					
Beamline	APS 24-ID-E	APS 24-ID-C	APS 24-ID-C	APS 24-ID-C	APS 24-ID-E
Wavelength (Å)	0.9792	1.6060	1.4857	1.2822	0.9792
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Cell dimensions					
a, b, c (Å)	80.74, 137.28, 150.16	81.16, 138.86, 149.88	81.24, 137.49, 149.56	80.91, 136.47, 150.07	81.11, 137.83, 149.76
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
Resolution	49.39 – 2.47 (2.53 – 2.47)	49.96 – 2.43 (2.49 – 2.43)	49.85 – 2.60 (2.68 – 2.60)	49.27 – 2.22 (2.26 – 2.22)	49.92 – 2.42 (2.48 – 2.42)
No. of unique reflections	60682 (4442)	64578 (4462)	52086 (4421)	82379 (4437)	64774 (4501)
$\langle I \rangle / \langle \sigma I \rangle$	15.8 (2.0)	22.7 (2.1)	15.9 (2.1)	15.7 (2.0)	14.8 (2.1)
R_{pim}	0.035 (0.330)	0.047 (0.337)	0.047 (0.326)	0.039 (0.443)	0.043 (0.335)
CC(1/2)	0.998 (0.763)	0.995 (0.745)	0.998 (0.762)	0.998 (0.737)	0.998 (0.773)
Redundancy	13.8 (12.8)	19.3 (19.4)	12.9 (13.9)	14.2 (13.8)	14.0 (14.0)
Completeness (%)	100.0 (100.0)	100.0 (100.0)	99.6 (99.2)	99.6 (98.7)	99.9 (100.0)
Wilson B-factor ($Å^2$)	57.0	64.4	53.1	44.2	47.6
Refinement					
Resolution (Å)	49.39 – 2.47	49.77 – 2.43	49.52 – 2.60	49.27 – 2.22	49.56 – 2.42
Rwork/Rfree	18.3/21.8	17.7/20.3	17.0/20.9	17.0/19.7	16.5/20.4
Rmsd from ideal geometry					
bond lengths (Å)	0.008	0.008	0.008	0.008	0.007
bond angles (°)	1.02	1.04	0.969	0.954	0.984
Ramachandran plot					
favored (%)	96.7	95.5	95.7	97.3	96.8
allowed (%)	3.3	4.4	4.1	2.7	3.2
outliers (%)	0.0	0.1	0.2	0.0	0.0
Average B-factor ($Å^2$)	61.5	77.5	67.9	50.2	59.2
Model contents					
Protomers/ASU	2	2	2	2	2
Protein residues	962	962	962	962	960
Ligands	4 Mn^{2+}, 2 GTP, 19 SO_4, 3 Cl, 2 sucrose	4 Co^{2+}, 2 GTP, 12 SO_4, 2 sucrose, 1 glycerol	5 Ni^{2+}, 2 GTP, 10 SO_4, 2 Cl 2 sucrose, 1 glycerol	4 Zn^{2+}, 2 GTP, 16 SO_4, 2 Cl, 2 sucrose, 2 glycerol	6 Cu^{2+}, 2 GTP, 19 SO_4, 2 Cl, 2 sucrose, 2 glycerol
Water	20	11	17	160	116
PDB ID	8DC9	8DCA	8DCB	8DCD	8DCF

Data for highest resolution shell are shown in parenthesis. Rfree was computed for ~ 5% of randomly selected reflections.

Table S2. Crystallographic data and refinement statistics.

Structure	PhoRtcB-(His234)-GMP
Data collection	
Beamline	APS 24-ID-C
Wavelength (Å)	1.8917
Space group	$P4_3$
Cell dimensions	
a, b, c (Å)	143.56, 143.56, 80.30
α, β, γ (°)	90, 90, 90
Resolution	47.85 – 2.35 (2.40 – 2.35)
No. of unique reflections	67599 (4104)
$\langle I \rangle / \langle \sigma I \rangle$	19.1 (2.2)
R_{pim}	0.033 (0.341)
CC(1/2)	0.999 (0.711)
Redundancy	12.6 (11.0)
Completeness (%)	99.0 (90.4)
Wilson B-factor (Å^2)	45.4
Refinement	
Resolution (Å)	47.85 – 2.35
Rwork/Rfree	19.1/21.7
Rmsd from ideal geometry	
bond lengths (Å)	0.008
bond angles (°)	0.961
Ramachandran plot	
favored (%)	96.9
allowed (%)	3.0
outliers (%)	0.1
Average B-factor (Å^2)	52.7
Model contents	
Protomers/ASU	2
Protein residues	962
Ligands	2 GMP, 25 SO_4, 4 Cl, 2 sucrose
Water	73
PDB ID	8DCG

Data for highest resolution shell are shown in parenthesis. Rfree was computed for ~5% of randomly selected reflections.