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Supporting information for article:

Structural and functional analysis of the RNA helicase Prp43 from the thermophilic eukaryote *Chaetomium thermophilum*

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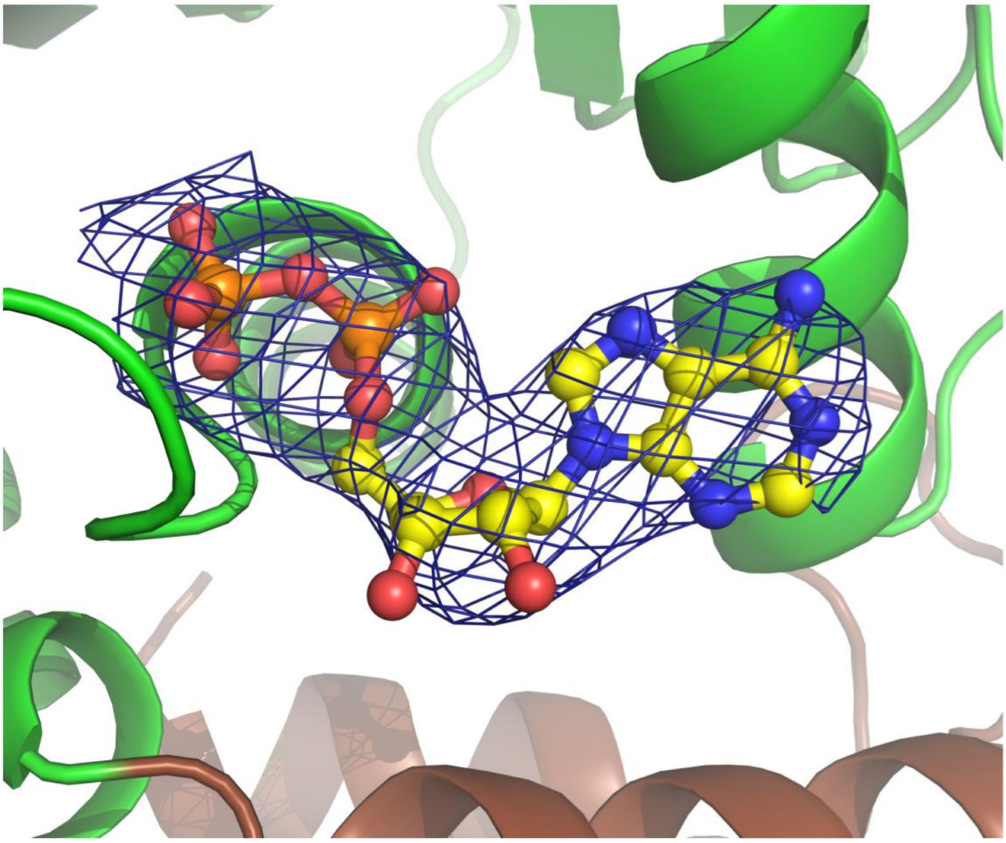

Figure S1 Omit map of ADP. The |Fo-Fc| electron density map contoured at 3 σ is depicted for the ADP molecule (shown as sticks and balls) bound to the active site of ctPrp43.

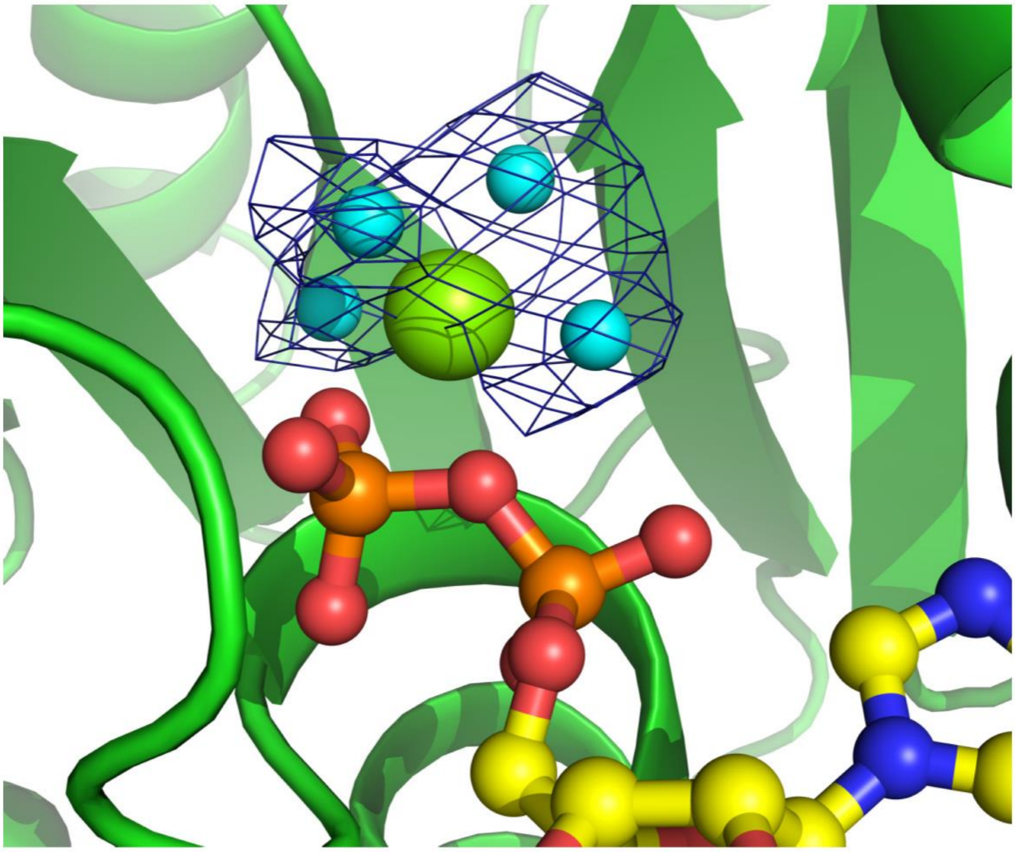

Figure S2 Omit map of the water molecules at the active site of ctPrp43. The |Fo-Fc| map contoured at 3 σ is shown for the four water molecules which are located at the active site. The water molecules are presented as cyan balls. The magnesium ion is depicted as larger light green ball but was not omitted for the |Fo-Fc| map calculation.

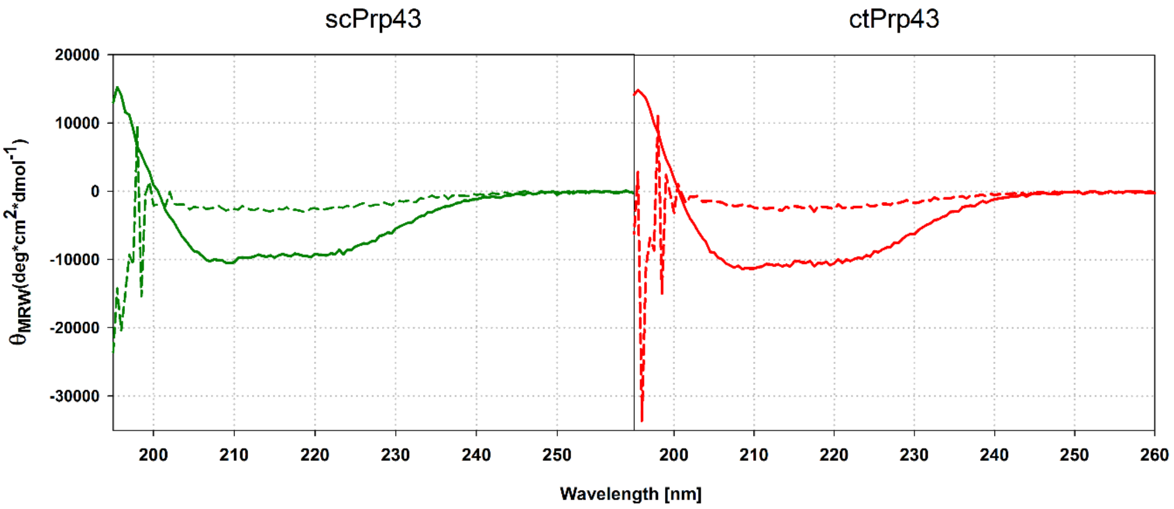

Figure S3 Far-UV spectra of ctPrp43 and scPrp43. CD-Spectra were recorded at 20°C (solid lines) and 84°C (dashed lines) between 195 nm to 260 nm. Curves acquired at 20°C show the characteristic curve progression for proteins containing β-sheets (maximum at 196 nm) and α-helices (maximum at 193 nm and minimum at 208 nm and 222 nm) as secondary structure elements. The 84°C sample unveils that protein denaturation occurred to a high degree.

Table S1 Distances of hydrogen bonds between ctPrp43 and the bound ADP or water molecules as well as the coordination distances of the central Mg^{2+}.

Interaction partner 1	Interaction partner 2	Distance (Å)
Gly 122 (N)	β-phosphate (O1B)	2.47
Gly 124 (N)	β-phosphate (O3B)	2.54
Lys 125 (N)	β-phosphate (O3B)	2.57
Lys 125 (NZ)	β-phosphate (O2B)	2.67
Thr 126 (OG1)	β-phosphate (O2B)	2.81
Thr 127 (N)	α-phosphate (O2A)	3.01
Thr 127 (OG1)	α-phosphate (O2A)	2.76
Asp 218 (OD2)	Water 4	2.85
Glu 219 (OE2)	Water 2	2.64
Glu 219 (OE2)	Water 3	2.62
Glu 219 (OE2)	Water 4	2.59
Asp 391 (OD2)	O2’ (Ribose ADP)	2.59
Asp 391 (OD1)	O2’ (Ribose ADP)	2.84
Arg 435 (NH2)	O3’ (Ribose ADP)	2.39
Water 1	α-phosphate (O1A)	2.95
Water 1	α-phosphate (O3A)	2.59
Water 3	β-phosphate (O2B)	2.79
Water 4	β-phosphate (O2B)	2.21
Mg^{2+}	Water 1	2.06
Mg^{2+}	Water 2	2.07
Mg^{2+}	Water 3	2.07
Mg^{2+}	Water 4	2.07
Mg^{2+}	β-phosphate (O2B)	2.07
Mg^{2+}	Thr 126 (OG1)	2.05

Table S2 Domain conservation between ctPrp43 and scPrp43.

	NTE	RecA-1	RecA-2	WH	Ratchet	OB-fold
Identity	29/109 (26.6 %)	142/176 (80.7 %)	149/190 (78.4 %)	55/66 (83.3 %)	64/116 (55.2 %)	71/136 (52.2%)
Similarity	53/109 (48.6 %)	158/176 (89.9 %)	170/190 (89.5 %)	59/66 (89.4 %)	86/116 (74.1 %)	92/136 (67.6 %)