SUPPLEMENTARY INFORMATION

The bacterial DNA sliding clamp, β-clamp: Structure, interactions, dynamics and drug discovery

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Supplementary figures and tables

Table S1: Structural alignment of β-clamps from different organisms[a]

PDB ID	Organism	Sequence identity	RMSD (Å)[b]	Sequence length
1MMI [33]	*Escherichia coli* (Gram-negative)	-	-	366
6AMQ [134]	*Enterobacter cloacae* (Gram-negative)	96%	0.97	366
6AMS [134]	*Pseudomonas aeruginosa* (Gram-negative)	56%	1.47	367
6AP4 [134]	*Acinetobacter baumannii* (Gram-negative)	46%	1.79	388
3P16 [135]	*Mycobacterium tuberculosis* (Gram-positive)	27%	1.96	408
4TR6 [76]	*Bacillus subtilis* (Gram-positive)	27%	1.85	380
2AVT [136]	*Streptococcus pyogenes* (Gram-positive)	23%	1.94	378
4S3I [79]	*Helicobacter pylori* (Gram-negative)	20%	1.92	384

[a]Alignments were done using the TM-Align algorithm [45], [b]RMSDs were calculated from the backbone C^{α} atoms of the superimposed structures.

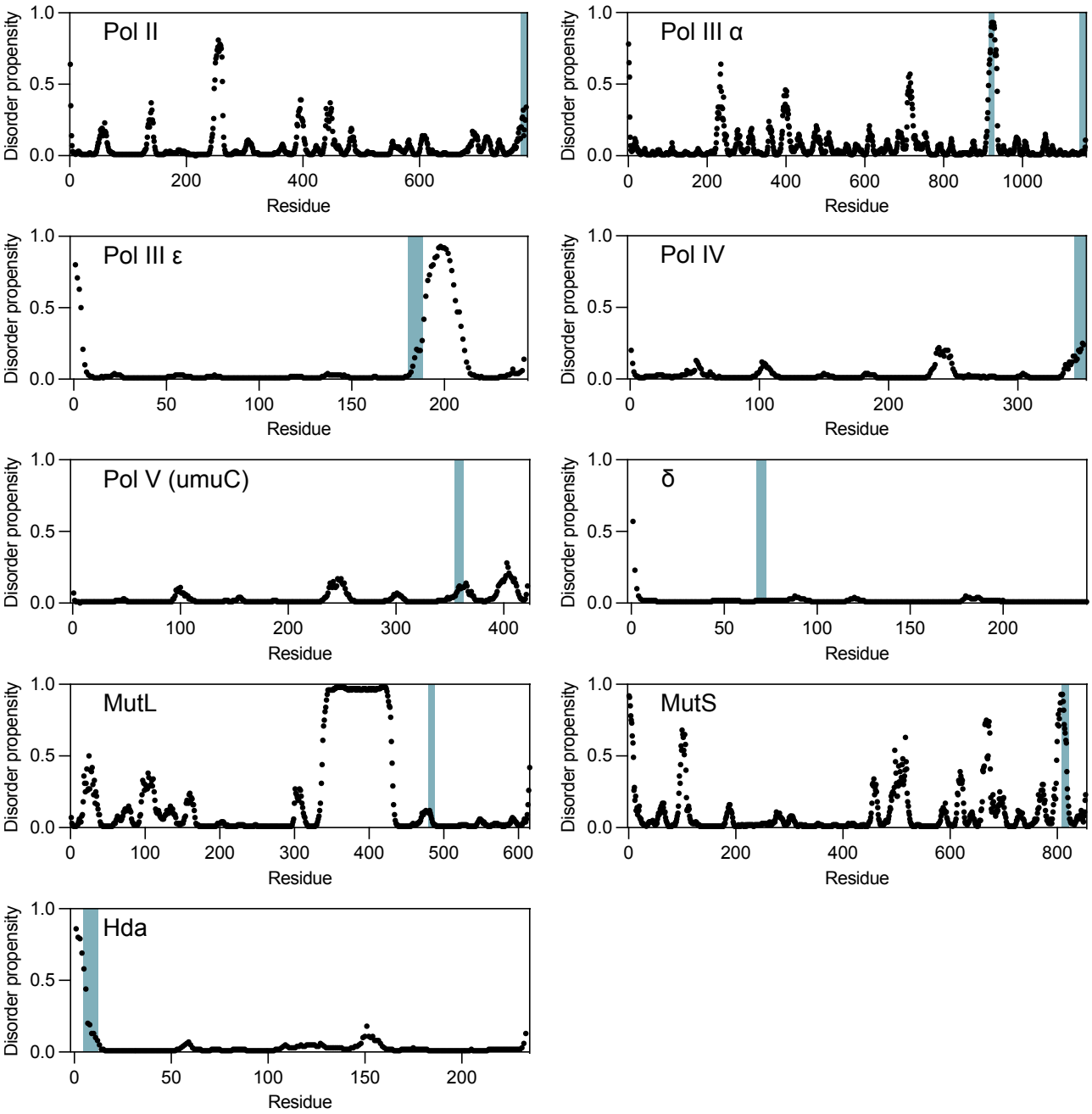

Fig. S1 Disorder prediction of selected β-clamp interaction partners. The disorder propensity is plotted for each residue and was predicted using DISOPRED3 (http://bioinf.cs.ucl.ac.uk/psipred) [137]. Blue boxes indicate the location of the β-clamp binding motifs (CBMs).

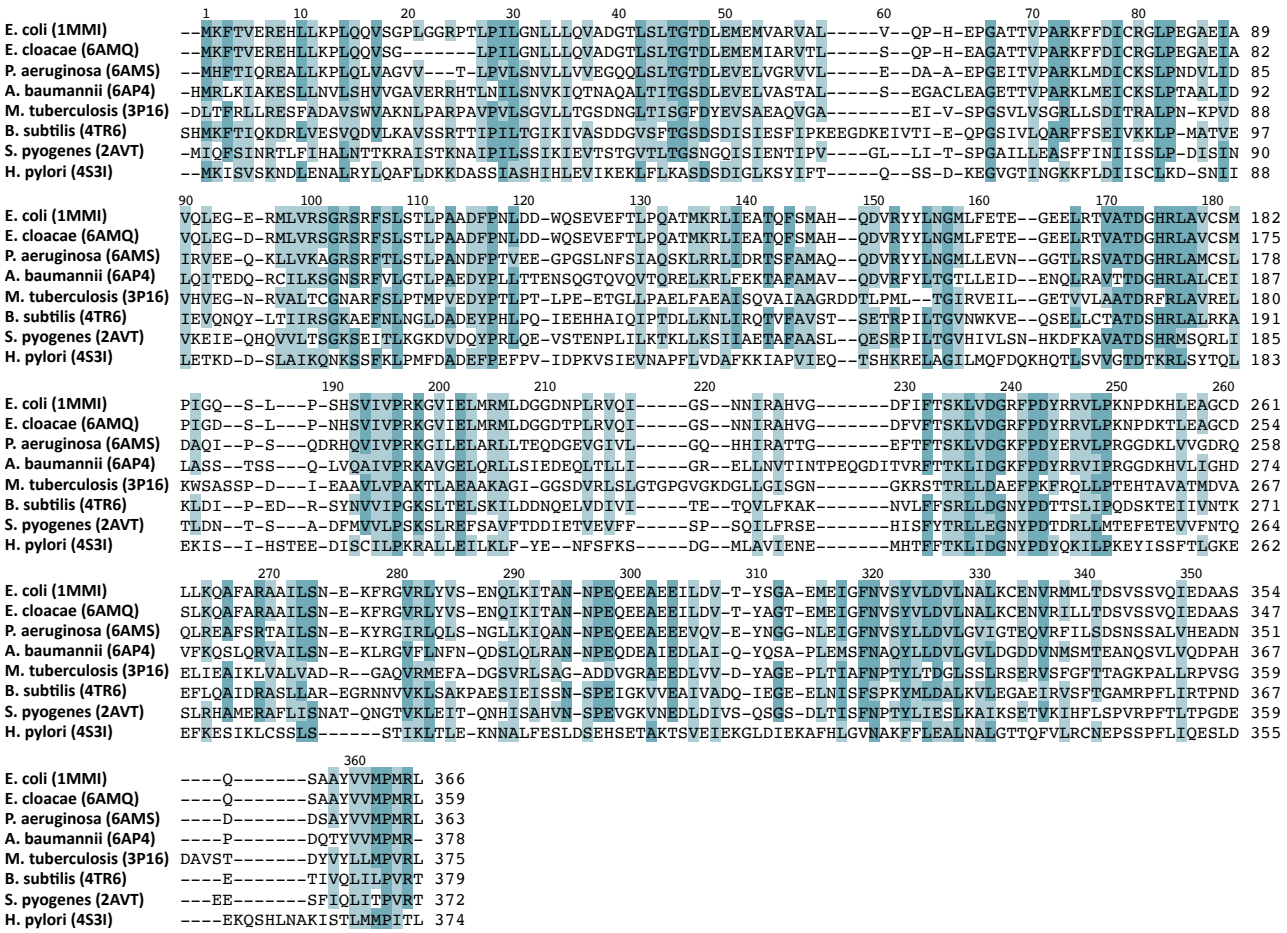

Fig. S2 Structural sequence alignment of β-clamps from different organisms. Sequence alignments are based on the structure alignment using the TM-align algorithm. Note that sequences not visible in the PDB structure are not present in this alignment. Sequence conservations are visualized using the Color Align Conservation tool at https://www.bioinformatics.org with a percentage identity or similarity cut-off of 70%. Amino acids are grouped according to their characteristics; positive = H, R ,K; negative = D, E; Neutral = S, T, N, Q; Aliphatic = A, V, L, I, M; Aromatic = F, Y, W; Pro & Gly = P, G; Cys = C. Numbers on top of the sequences are amino acid positions of the E. coli β-clamp sequence

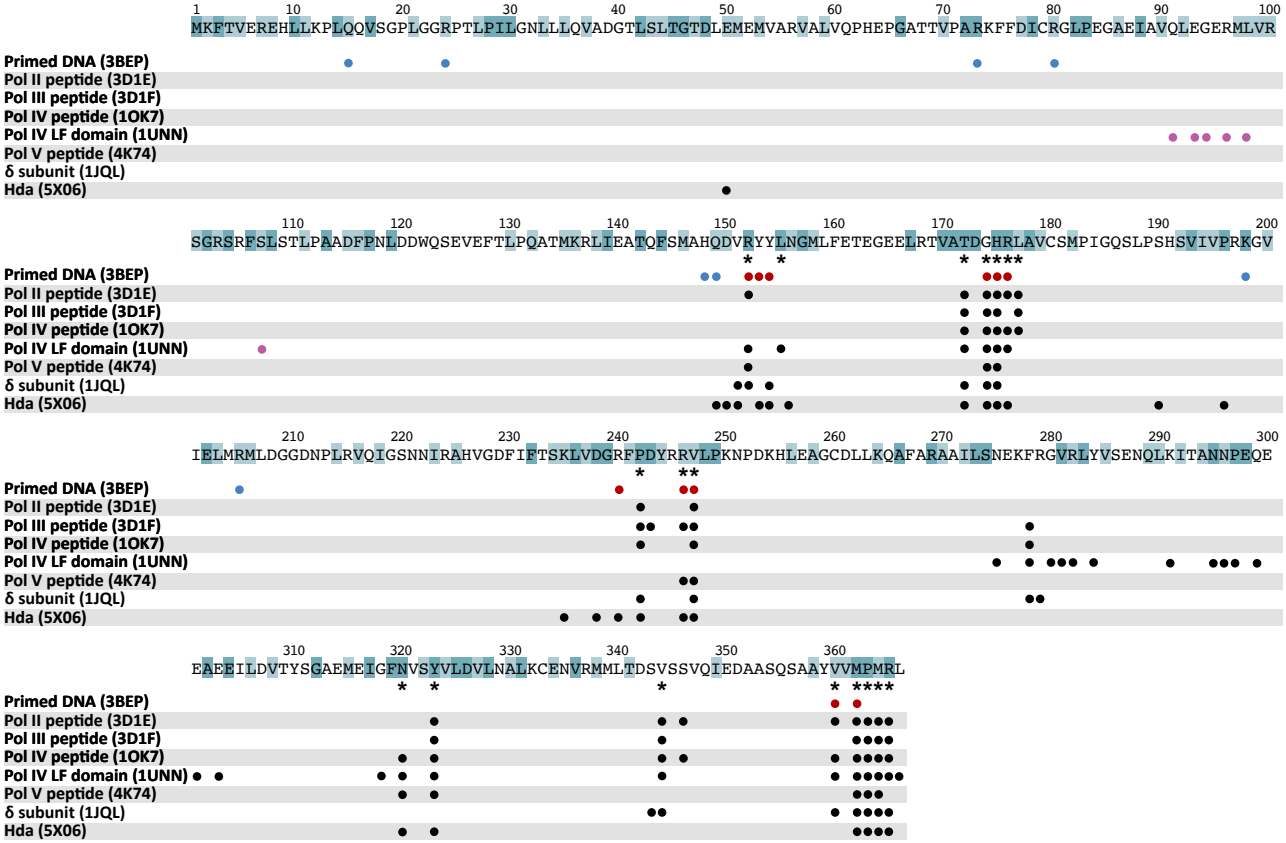

Fig. S3 Overview of β-clamp interacting residues and their conservation. PDBsum [138] was used to identify β-clamp residues that are in close proximity (≤ 3.9 Å) to the protein or peptide interaction partners (PDB ID in the parenthesis) in the crystal structures (black dots). The interacting residues between β-clamp and primed DNA are based on the interactions reported in the paper by Georgescu et al. [5]. β-clamp residues are coloured according to their structural sequence conservation as shown in Fig. S2. Stars indicates residues that constitute the canonical CBM binding pocket. Blue dots of the primed DNA interaction indicate interactions with the inner hole of β-clamp and red dots indicate interactions to residues of an adjacent β-clamp molecule in the crystal lattice. Purple dots of the Pol IV LF domain interaction indicate interactions formed by the other subunit of the β-clamp dimer.