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Supplemental Information

**A Comparative Structure/Function Analysis of Two
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a Novel Mode of DNA Binding**

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A comparative structure/function analysis of two type IV pilin DNA receptors defines a novel mode of DNA-binding

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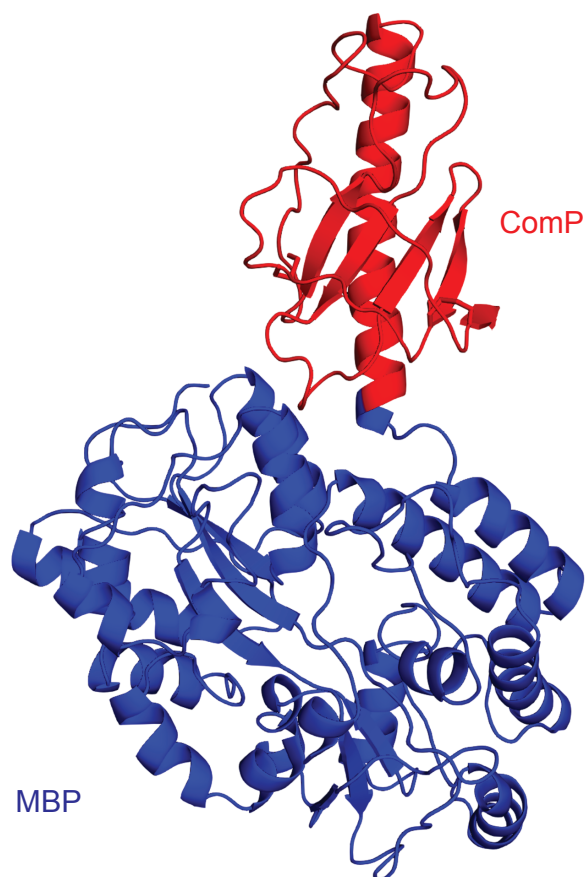


Figure S1, related to Figure 3. Full 3D structure of the MBP-ComP fusion protein. The crystal structure is shown as a cartoon drawing. The ComP moiety is highlighted in red, while the MBP moiety is highlighted in blue.

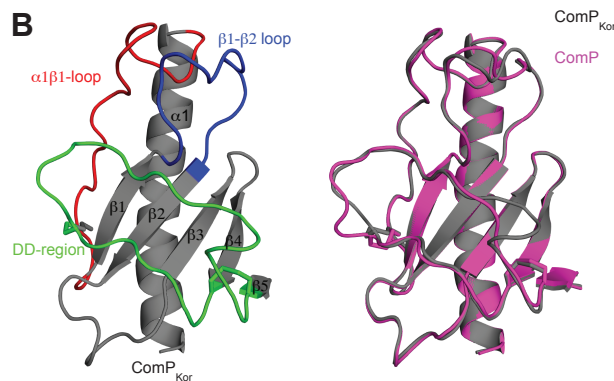
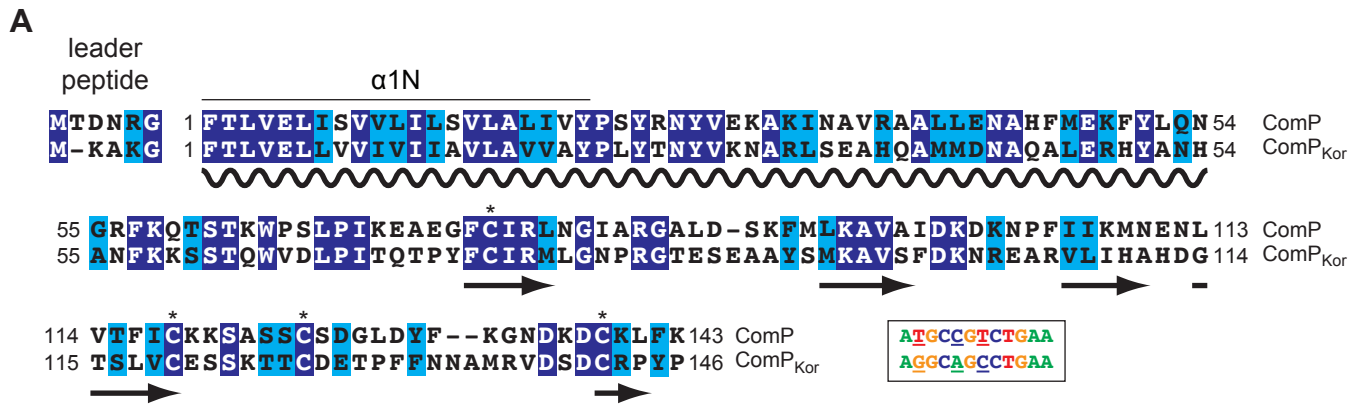


Figure S2, related to Figures 3 and 4. Homology modelling of the structure of the ComP_{Kor} ortholog from *K. oralis*. (A) Sequence alignment of ComP_{Kor} with ComP from *N. meningitidis* 8013, produced using Clustal Omega. Amino acids were shaded in dark blue (when identical), in light blue (when highly similar) or non-shaded (when non-conserved). Relevant structural and functional features have been highlighted. The four Cys residues that form two crucial disulfide bonds are identified by *. The inset represents a sequence alignment of DUS and the DUS variant found in *K. oralis*. These motifs differ by three base, which have been underlined. (B) Cartoon drawing representation of the homology model of ComP_{Kor} and of its superposition with the ComP crystal structure.

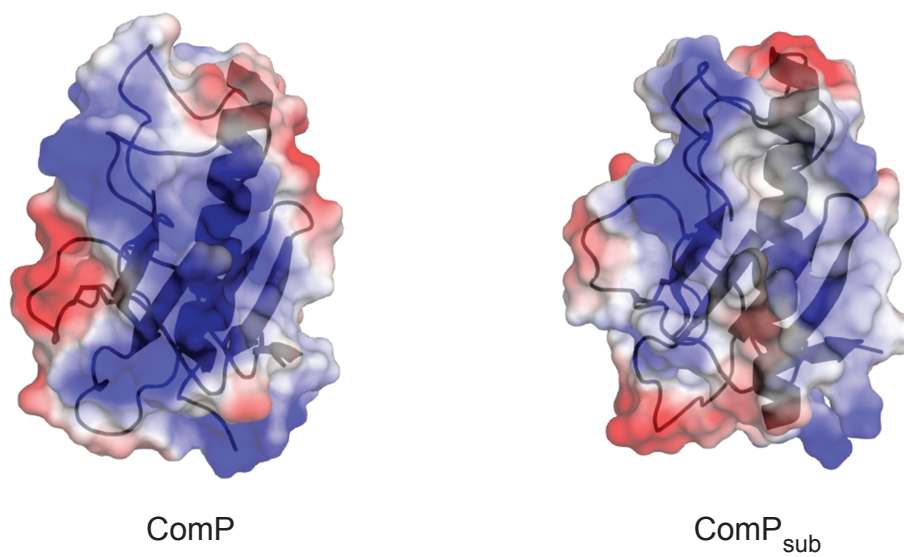


Figure S3, related to Figures 3 and 4. Surface charge representation of the ComP and ComP_{sub} structures. Positively charged residues are represented in blue, negatively charged residues in red, while neutral residues are not coloured.

Table S1, related to Figures 3 and 4. Structural data collection and refinement parameters.

MBP-Comp		
Resolution range (Å)	58.05-1.43 (1.47-1.43)	
Space group	$P2_12_12_1$	
Unit cell dimensions	63.57, 68.44, 109.58; 90, 90, 90	
Total observations	415,797 (28,880)	
Total unique	88,446 (6,445)	
Multiplicity	4.7 (4.5)	
Completeness (%)	99.5 (99.2)	
$I/\sigma(I)$	15 (1.2)	
Wilson B factor		21.3
R_{merge}	0.039 (1.096)	
R_{meas}	0.049 (1.384)	
R_{work}		0.16
R_{free}		0.19
Ramachandran favoured (%)		97.2
Ramachandran outliers (%)		0
Average B factor		29
His₆-Comp_{sub}		
Number of distance restraints		2,017
intra-residual		744
sequential		445
medium range		273
long range		555
NOE violations >0.5 Å		1
Dihedral violations >5°		0
Ramachandran favoured (%)		75.5
Ramachandran allowed (%)		20.6
Ramachandran generously allowed (%)		3.9
Ramachandran disallowed (%)		0

Table S2, related to the Experimental procedures. Primers used in this study.

Name	Sequence^a
Cloning	
<i>optcomP</i> -F	gggaattc GAAAAAGCCAAAATTAACGCAGTT
<i>optcomP</i> -R	ggaagctt TTATTTAAACAGTTTGCAGTCTTTG
<i>comP</i> _{sub} -pMalF	gggaattc CGCTCGGCCAACCTGCGTG
<i>comP</i> _{sub} -pMalR	ggaagctt TCACCCCGTAAAAGGCCGA
<i>hiscomP</i> _{sub} -pETF	ggccatgg atcatcatcatcatcatcatCGCTCGGCCAACCTGCGTG
<i>hiscomP</i> _{sub} -pETR	ccggatcc TCACCCCGTAAAAGGCCGA
DNA-binding assay (EMSA/SPR)	
DUS _{var1} 1 ^b	tgacc AGGCCGTCTGAA caaac
DUS _{var1} 2	gtttg TTCAGACGGCCT ggtca
SUD1 ^b	tgacc ACGACTTATAAT caaac
SUD2	gtttg ATTATAAGTCGT ggtca
SDU1 ^b	tgacc AAGGCCTGTCAT caaac
SDU2	gtttg ATGACAGGCCTT ggtca
NMR titration	
DUS _{var1} 1bis	cAGGCCGTCTGAA c
DUS _{var1} 2bis	gTTCAGACGGCCT g

^aOverhangs are in lower case, with restriction sites in bold.

^bWhen indicated, these primers were 5'-labelled with biotin.