Electronic Supplementary Material (ESI) for Molecular BioSystems.

Table S1: List of all PDB ID used in the study.

PDB ID	No. of H-Bond	Resolution	PDB ID	No. of H-Bond	Resolution	PDB ID	No. of H-Bond	Resolution
2G1P	7	1.89	**1TEZ**	11	1.8	**3FDE**	4	1.41
3NDH	16	1.3	**4JWM**	8	2	**4MDF**	13	1.73
1DFM	5	1.5	**3FSI**	6	1.75	**3O3F**	2	2
1KX3	53	2	**4KLI**	11	1.6	**1XO0**	27	2
2Z70	2	1.7	**4KB1**	4	1.8	**3U7F**	0	1.8
3FC3	29	1.75	**1RXW**	5	2	**2R1J**	21	1.53
1KX3	53	2	**4JCY**	13	1.8	**1JB7**	0	1.86
3MXM	4	1.75	**4HCB**	14	2	**3PV8**	18	1.52
1UUT	14	2	**3QN0**	0	2.34	**2VLA**	9	1.3
3DVO	51	1.89	**1NH2**	0	1.9	**1NH2**	0	1.9
3PVI	0	1.59	**2BCQ**	15	1.65	**3SPD**	12	1.91
1MW8	10	1.9	**1OMH**	9	1.95	**4LJR**	1	1.8
3ZDB	2	1.47	**3M4A**	8	1.65	**4GJR**	24	1.85
3VOK	0	2	**4E9F**	7	1.79	**3PVV**	15	2
3RAX	9	1.89	**1ORN**	9	1.7	**2D5V**	36	2
2ODI	1	1.45	**2GIG**	6	1.83	**4NDH**	7	1.85
1JB7	0	1.86	**4K1G**	2	1.9	**1TRO**	35	1.9
1FIU	30	1.6	**3VAJ**	0	1.9	**2DP6**	11	1.8
4G92	21	1.8	**1CYQ**	4	1.93	**4LZG**	18	1.6
1NH2	0	1.9	**2FR4**	0	1.95	**1NKP**	36	1.8
4GLX	16	1.9	**4HJE**	8	1.91	**2W42**	11	1.9
1SXQ	4	1.8	**1DC1**	17	1.7	**3Q23**	7	1.8
4AIK	5	1.85	**1Y8Z**	2	1.9	**1H6F**	5	1.7
2C7Q	2	1.85	**4J2D**	2	1.76	**1F0V**	1	1.7
1LMB	9	1.8	**2WIW**	0	1.8	**4GZ1**	5	1.5
3AAF	6	1.9	**4HLY**	8	1.48	**4IX7**	20	1.58
1T9I	6	1.6	**2W7N**	41	1.85	**4M3Z**	2	1.84
4LUP	8	1.2	**1MUS**	6	1.9	**1K3X**	0	1.25
1WTE	38	1.9	**2I13**	55	1.96	**2IH2**	8	1.61
4O6A	9	1.86	**1SA3**	0	1.95	**3OSG**	24	2
2AXY	10	1.7	**4B21**	6	1.45	**2XZF**	1	1.8
3BEP	1	1.92	**3QEX**	4	1.73	**3FDQ**	5	1.75
1OE4	6	2	**4I2O**	20	1.77	**2XHI**	12	1.55
4ECQ	9	1.5	**2VE9**	42	1.9	**2E52**	16	2
2AC0	8	1.8	**1KX3**	53	2	**2A07**	23	1.9
2OFI	3	1.85	**2H7G**	9	1.9	**2OAA**	1	1.5
1L3L	32	1.66	**1NH2**	0	1.9	**4G92**	21	1.8
4IBU	14	1.7	**4C8M**	10	1.57	**4JRP**	20	1.95
3OQG	36	1.75	**1KX3**	53	2	**2XQC**	18	1.9
2NQ9	0	1.45	**4M95**	4	1.72	**3UBY**	7	2
2PY5	12	1.6	**4I2A**	0	1.9	**4NDI**	7	1.9
3GA6	5	1.9	**3BAM**	1	1.8	**3K59**	8	1.92
3SM4	11	1.88	**3G0X**	0	1.8	**2FR4**	0	1.95
1RFF	2	1.7	**4BWJ**	15	1.55	**3JXY**	12	1.5
3BM3	0	1.7	**4J2A**	2	1.8	**1CL8**	2	1.8
4K98	6	1.94	**1LAU**	1	1.8	**1SX5**	3	1.5

Table S2: Effect of secondary structure of Mtb-SigH on MD simulation on interaction with 20 different promoters. The secondary structure of Mtb-SigH before MD simulation (initial) is used as control. The complexes showing satisfactory interaction is marked in red, the average interacting complex is shown in blue and the poor interacting ones are demarcated in orange. The table also includes the amino acid sequence of Mtb-SigH.

Complex	Secondary structure
Initial	CHHHHHHHHHHHHCCCHHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHHCCCCCCCCCCCHHHHHHHHHHHHH
PsigL	CHHHHHHHHHCCCHHHHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHHCCCCCCCCCCCHHHHHHHHHHHHH
PctpB	CHHHHHHHHCCCCCCCHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHHCCCCCCCCCCCHHHHHHHHHHHHH
PsigH	CCHHHHHHHHHHCHHHHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHHCCCCCCCCCCCHHHHHHHHHHHHH
PrrnA	CCHHHHHHHHCCCCCCHHHHHHHHHHHHCCCHHHHHHHHHHHHHHHHCCCCCCCCCCCCHHHHHHHHHHHHH
PSinP3	CHHHHHHHHHHHHCCCHHHHHHHHHHHHCCCCHHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHCC
Plac cons	CCHHHHHHHHHHHCCCHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHHH
PsigD	CCHHHHCCCCCCCCCHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHHH
PrshA	CHHHHHHHHHHHHHHHHHHCHHHHHHHHCCHHHHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHHH
PsigI	CCCHHHHHHHCCCCCCHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHHCCCCCCCCCHHHHHHHHHHHHC
PRrs2	CCHHHHHHHHHHCHHHHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHH
PlexA	CCCCHHHHHHHHHCCHHHHHHHHHHHHCCCCHHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHH
P16S	CCHHHHHHHHHCCCCHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHH
PesxE	CCCHHHHHHHHCCHHHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHH
PusfX	CHHHHHHHCCCCCCCHHHHHCHHHHHCCHHHHHHHHHHHHHHHCCCCCCCCCCHHHHHHHHHHHHC
Phsp20	CHHHHHHHHHHCCCCHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHCCCCCCCCCHHHHHHHHHHHH
PsigH1	CHHHHHHHHCCCCCCHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHCCCCCCCCCHHHHHHHHHHHH
PN25	CHHHHHHHHHHHCCCHHHHHHHHHHHHCCHHHHHHHHHHHHHHHHCCCCCCCCCHHHHHHHHHHHH
PN25 cons	CCCCHHHHHCCCCCCHHHHHHHHHHCCCHHHHHHHHHCHHHHHHHHCCCCCCCCCHHHHHHHHHHHH
PPCL1	CHHHHHHHHHHHCCCHHHHHHHHHHHCCCCCHHHHHHHHHHHCCCCCCCCCHHHHHHHHHHHH
PmmR	CHHHHHHHHHHHCCCHHHHHHHHHHHCCHHHHHHHHHHHHHHHCCCCCCCCCHHHHHHHHHHHH
Sequence	TDEELTARFERDAIPLLDQLYGGALRMTRNPADAEDLLQETMVKAYAGFRSFRHGTNLKAWLYRILTNTYINSYR
	1 1 1 1 1 1 1 1

Table S3: Hydrogen bond analysis between Mtb-SigH with the various promoters

Promoter	Number of stable H-bonds including phosphate group	Highest occupancy residue name	Number of stable H-bonds involving DNA bases	Atoms involved in sequence specific H-bonds
PrrnA	8	ARG 64 HH12:ADE 9 O1P	3	ASN 72 HD21:ADE 36 N7 ASN 72 HD21:THY 37 O4 ASN 72 HD22: ADE 36 N7
PmmR	5	ARG 64 HH21: THY 8 O1P	NIL	-
PctpB	15	ARG 64 HE:CYT 9 O2P	5	ASN 68 HD21:GUA 10 N7 ASN 68 HD21:ADE 11 N7 ASN 72 HD22:ADE 38 N7 ASN 72 HD22:GUA 39 06 ASN 72 HD22:ADE 11 N7
PsigD	6	ASN 68 HD22:GUA 10 O2P	1	ASN 68 HD21:GUA 10 N7
PsigH	5	SER73 HG1:THY 36 O2P	NIL	-
Phsp20	10	ARG 64 HH22:GUA 8 O1P	NIL	-
P16S	10	SER 73 HG1:CYT 38 O2P	1	ASN 72 HD22:ADE 39 N7
PusfX	14	SER 73 HG1:ADE 40 O2P	5	ASN 68 HD21:GUA 10 N7 ASN 72 HD22:THY 11 O4 ASN 72 HD22:ADE 40 N7 ASN 72 HD22:THY 41 O4 ASN 72 HD21: THY 41 O4
PsigI	9	THR 67 HG1:THY 10 02P	5	ASN 68 HD21:GUA 38 O6 ASN 72 HD21:ADE 36 N7 ASN 72 HD21:GUA 37 O6 ASN 72 HD22: GUA 37 O6 ASN 72 HD22:GUA 37 N7
PesxU	12	ASN 72 OD1:ADE 37 H61	1	ASN 72 HD 22:ADE 37 N7
PSinP3	11	SER 73 HG1: ADE 38 O2P	3	ASN 72 HD21:ADE 11 N7 ASN 72 HD21:THY 29 O4 ARG 75 HH12: THY 37 O2P
Plac cons	8	ARG 75 HH11:THY 37 O2P	2	ASN 72 HD 21:ADE 40 N7 ASN 72 HD 21:THY 41 O4
PRrsp2	17	ARG 75 HH12:CYT 37 O2P	6	ASN 72 HD 21:GUA 11 O6 ASN 72 HD 21:GUA 39 O6 ASN 72 HD 21:GUA 39 N7 ASN 72 HD 22:ADE 38 N7 ASN 72 HD 22:GUA 39 O6 ASN 72 HD 22:GUA 39 N7
PlexA	8	ARG 64 HH12:CYT 9 O1P	NIL	-
PN25	9	ARG 64 HH22:ADE 8 O1P	3	ASN 72 HD 22:THY 11 O4 ASN 72 HD 22:ADE 56 N7 ASN 72 HD 22:ADE 57 N7
PN25 cons	7	ARG 64 HE:ADE 9 O1P	1	ASN 72 HD22:ADE 53 N7
PPCL1	14	ASN 72 HD21:GUA 52 N7	3	ASN 72 HD21:GUA 52 O6 ASN 68 HD21:ADE 10 N7
PsigH1	12	ARG64 HH12:ADE9 O2P	3	ASN 68 HD21:GUA 10 N7 ASN 72 HD21:ADE40 N7 ASN 72 HD21: THY 41 O4
PrshA	11	ARG 64 HH22:THY8O1P	NIL	-
PsigL	11	ARG 75 HH11:THY 33 O2P	11	ASN 68 HD21:GUA 11