Supplementary Material

Structural determinants of specific DNA-recognition by the THAP zinc finger

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Supplementary Figure 1. ^{15}N longitudinal (R_1) and transverse (R_2) relaxation rates along the sequence for the THAP zinc finger of THAP1 in its DNA-bound state. Secondary structure elements are shown on the above panel.

Supplementary Figure 2. Influence of ionic strength on nonspecific DNA binding. **(A)** Plot showing the evolution of fluorescence anisotropy of Trp36 as a function of increased DNA at 250 (green), 150 (blue) and 30 (red) mM NaCl. **(B)** Overlay of 2D ^{1}H-^{15}N HSQC spectra of the protein in the absence (black) and in the presence of nonspecific DNA at 250 (green), 150 (blue) and 30 (red contour levels) mM NaCl. Residues that undergo chemical shift change of their backbone amide nitrogen upon decreasing NaCl concentration are indicated.

Supplementary Table 1. Intermolecular NOEs extracted from 3D ^{15}N HSQC NOESY, 3D $^{13}C_{ali}$ HSQC NOESY and 3D $^{13}C_{aro}$ HSQC NOESY.

Supplementary Table 2. Hydrogen bonds observed in the NMR structure of the complex formed by the THAP zinc finger of THAP1 and the 16 bp rrm1 DNA target.

Supplementary Table 3. Hydrophobic contacts observed in the NMR structure of the complex formed by THAP zinc finger of THAP1 and the 16 bp rrm1 DNA target.

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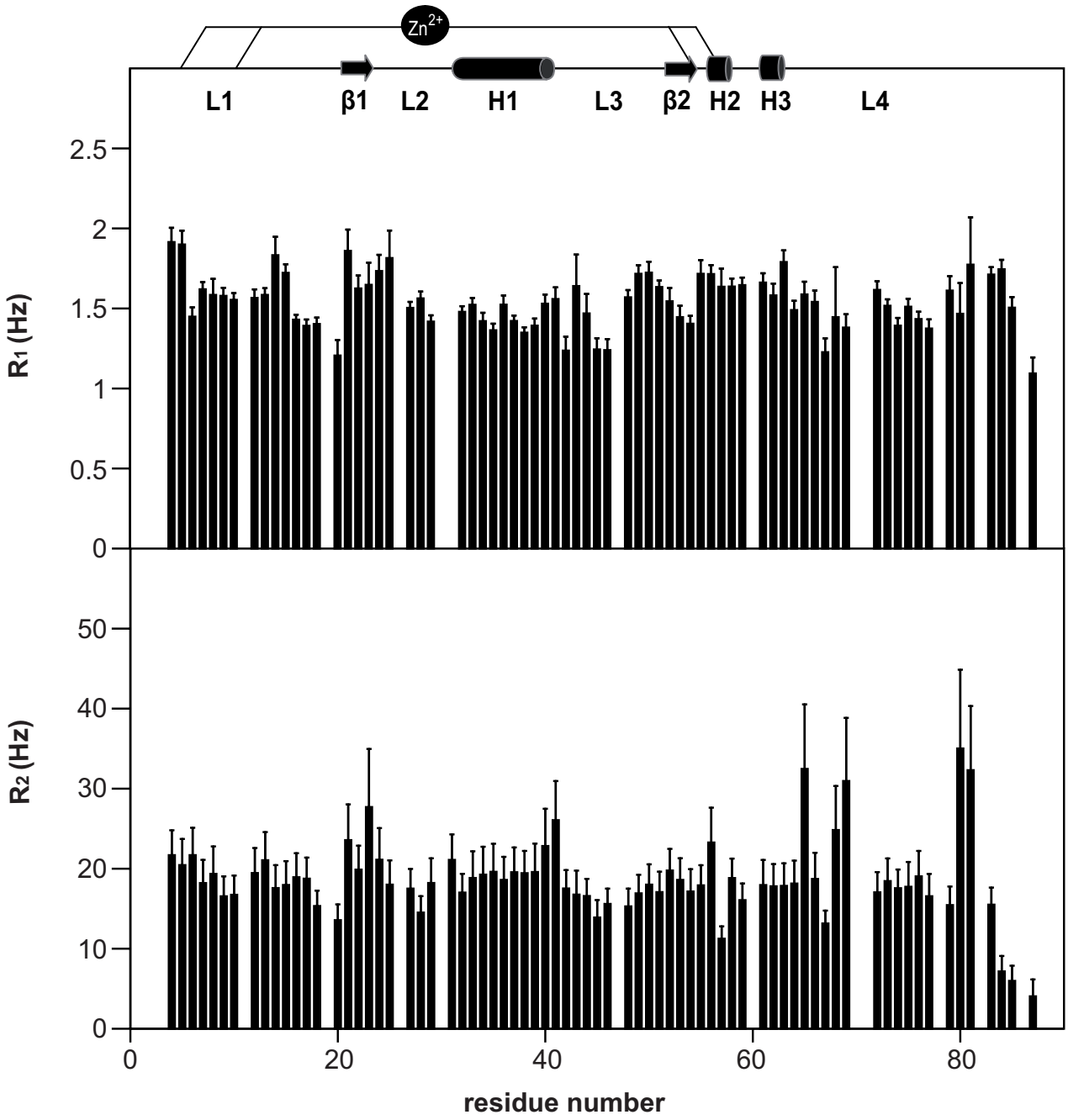
Supplementary Figure 1



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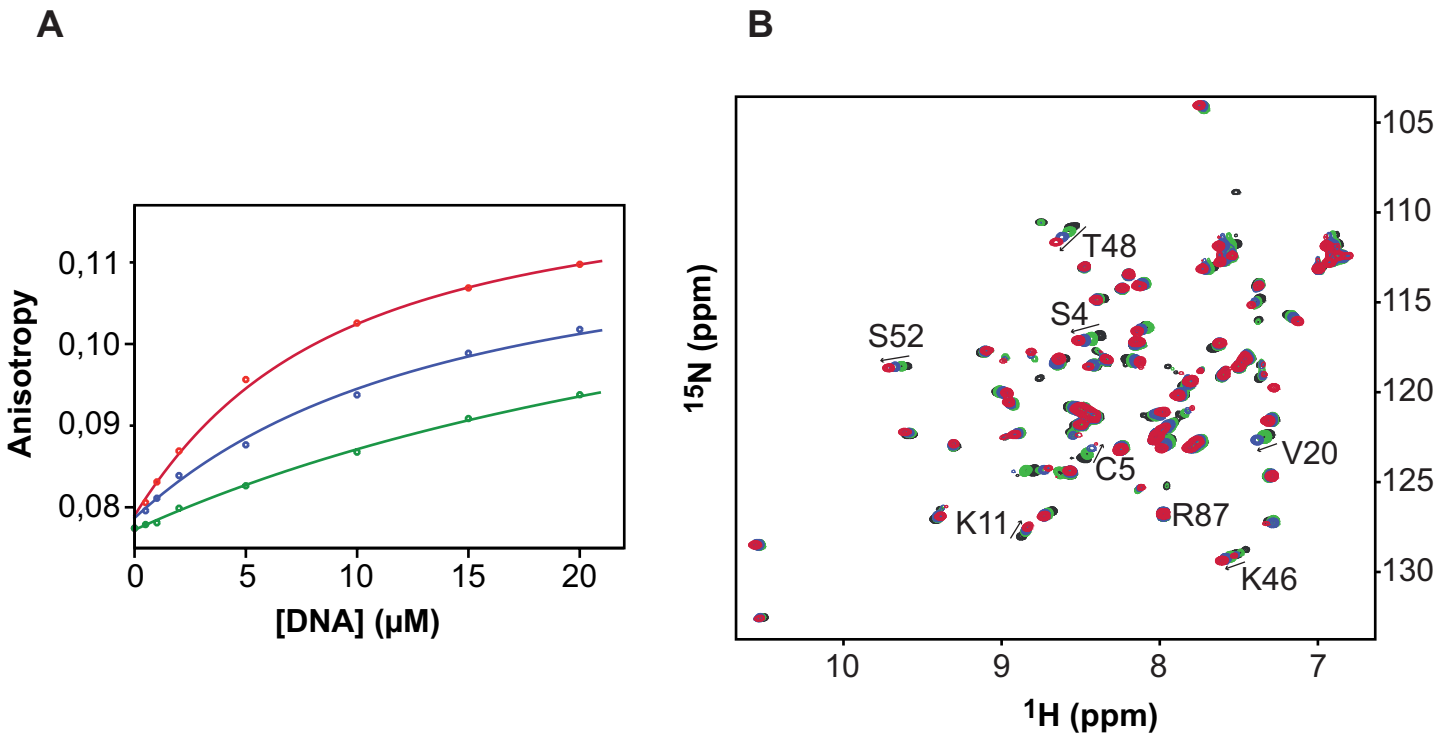
Supplementary Figure 2



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Supplementary Table 1

Amino acid atom	Nucleic acid atom	Interaction strength
H_N Lys 24	$H_{2'}$ Thy 8	low
	$H_{3'}$ Thy 8	low
	$H_{5''}$ Thy 8	low
H_β Asn 44	$H_{4'}$ Cyt 19	low
H_α Pro 47	H_{41} Cyt 22	medium
	H_5 Cyt 22	low
	H_6 Cyt 22	low
H_N Thr 48	H_{41} Cyt 22	strong
	H_5 Cyt22	medium
	H_6 Cyt 22	low
	H_8 Gua 21	strong
	H_5 Cyt 22	medium
H_α Thr48	H_5 Cyt 22	medium
H_β Thr48	H_5 Cyt 22	strong
$H_{\gamma 2}$ Thr48	H_{41} Cyt 22	medium
	H_6 Cyt 22	low
	$H_{3'}$ Gua 21	strong
	$H_{4'}$ Gua 21	low
H_N Lys 49	H_5 Cyt 22	low
H_N Tyr 50	H_5 Cyt 22	strong
H_α Tyr 50	H_5 Cyt 22	low
	H_5 Cyt 23	low
	H_6 Cyt 23	low
$H_{\beta 1}$ Tyr 50	H_5 Cyt 22	low
	H_5 Cyt 23	medium
$H_{\beta 2}$ Tyr 50	H_5 Cyt 22	medium
	H_5 Cyt 23	medium
H_N Ser 51	H_5 Cyt 22	medium
	H_{41} Cyt 22	strong
	H_6 Cyt 22	low
H_α Ser 51	H_{41} Cyt 22	strong
	H_6 Cyt 22	low
	H_{42} Cyt 22	medium
H_β Ser 51	H_{41} Cyt 22	medium
	H_6 Cyt 22	low
H_δ Arg 65	H_2 Ade 27	low
$H_{\delta 2}$ Leu 71	$H_{1'}$ Gua 7	long
	$H_{3'}$ Gua 7	medium

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Supplementary Table 2

Hydrogen bonds

Protein	Atom	Base	Atom	Distance (Å)	No (of 15)
Gln3	OE	CYT12	H41	2.08 ± 0.09	15
Gln3	HE2*	THY20	O4	2.15 ± 0.05	15
Lys11	HZ*	CYT19	O1P	1.85 ± 0.15	15
Arg13	HH1*	GUA10	O1P	2.08 ± 0.21	3
Arg13	HH2*	GUA11	O2P	2.23 ± 0.00	3
Tyr14	HH	GUA9	O1P	1.81 ± 0.11	15
Phe22	HN	GUA9	O2P	2.44 ± 0.04	2
Lys24	HN	THY8	O2P	2.08 ± 0.08	15
Lys24	HZ*	THY8	O4	2.37 ± 0.10	15
Lys24	HZ*	GUA9	O6	2.19 ± 0.02	14
Thr28	HG1	GUA7	O1P	1.82 ± 0.04	15
Lys46	HZ*	THY20	O1P	2.24 ± 0.16	5
Lys46	HZ*	THY20	O2P	1.92 ± 0.11	15
Thr48	HG1	CYT22	O2P	1.86 ± 0.05	15
Tyr50	O	CYT23	H41	1.92 ± 0.03	15
Tyr50	HH	CYT23	O2P	2.04 ± 0.08	15
Ser51	OG	CYT22	H41/H42	2.32 ± 0.10	6
Ser52	HG	GUA10	N7	2.28 ± 0.03	14
Lys64	HZ*	THY8	O2P	1.86 ± 0.12	12
Arg65	HH1*	THY6	O2	2.48 ± 0.00	1
Arg65	HH1*	GUA7	O4’	1.95 ± 0.03	15
Lys70	HZ*	ADE29	O3’	1.99 ± 0.22	10
Lys70	HZ*	ADE30	O1P	2.35 ± 0.09	4

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Supplementary Table 3

Hydrophobic contacts

Protein	Atom	Base	Atom	Distance (Å)	No (of 15)
Lys24	CB	THY8	C7	3.65 ± 0.10	14
	CG	THY8	C7	3.45 ± 0.09	3
	CD	THY8	C7	3.55 ± 0.12	11
	CE	THY8	C7	3.63 ± 0.10	10
Thr28	CG2	THY6	C3’	3.72 ± 0.18	11
Pro47	CA	THY20	C2’	3.69 ± 0.10	14
	CA	GUA21	C8	3.84 ± 0.03	9
	CB	GUA21	C8	3.70 ± 0.05	12
	CG	THY20	C2’	3.83 ± 0.06	12
	CG	THY20	C6	3.82 ± 0.05	6
	CD	THY20	C2’	3.85 ± 0.05	9
Thr48	CG2	GUA21	C2’	3.37 ± 0.05	15
	CG2	GUA21	C3’	3.56 ± 0.03	15
Tyr50	CB	CYT22	C4	3.73 ± 0.06	15
	CB	CYT22	C5	3.20 ± 0.02	15
	CB	CYT22	C6	3.32 ± 0.02	15
	CB	CYT23	C4	3.88 ± 0.01	7
	CB	CYT23	C5	3.57 ± 0.03	15
	CD1	CYT22	C2’	3.84 ± 0.04	10
	CD1	CYT23	C5	3.14 ± 0.02	15
	CD1	CYT23	C6	3.85 ± 0.02	13
	CD2	CYT22	C2’	3.15 ± 0.03	15
	CD2	CYT22	C5	3.63 ± 0.03	15
	CD2	CYT22	C6	3.08 ± 0.03	15
	CE1	CYT22	C2’	3.81 ± 0.04	9
	CE2	CYT22	C2’	3.13 ± 0.03	15
	CE2	CYT22	C3’	3.84 ± 0.04	14
	CG	CYT22	C2’	3.55 ± 0.03	15
	CG	CYT22	C5	3.83 ± 0.02	15
	CG	CYT22	C6	3.46 ± 0.02	15
	CG	CYT23	C5	3.62 ± 0.04	15
	CZ	CYT22	C2’	3.50 ± 0.04	15
Arg65	CD	GUA7	C4’	3.38 ± 0.11	15