Supplementary Data

Characterization of the interaction interface and conformational dynamics of human TGIF1 homeodomain upon the binding of consensus DNA

Shuangli Li[1, 2], Rui Hu[1], Haijie Yao[3], Dong Long[3, 4], Fan Luo[1], Xin Zhou[1], Xu Zhang[1], Maili Liu[1], Jiang Zhu[1,*], and Yunhuang Yang [1,*]

[1] State Key Laboratory of Magnetic Resonance and Atomic Molecular Physics, National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Chinese Academy of sciences, Wuhan, 430071, China.

[2] Graduate University of Chinese Academy of Sciences, Beijing, 100049, China.

[3] School of Life Sciences, University of Science and Technology of China, Hefei, 230027, China.

[4] Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, 230027, China.

* Correspondence to:

Jiang Zhu, E-mail: jiangzhu@wipm.ac.cn or Yunhuang Yang, Phone: +86-27-87199541, Fax: +86-27-87199543; E-mail: yang_yh@wipm.ac.cn.

Table. S1 Chemical shift assignments of backbone ^{1}H-^{15}N from 28 residues in the holo-TGIF1-HD based on NMR backbone assignment experiments, and the corresponding $\Delta\omega_{direct}$ and $\Delta\omega_{CEST}$.

Secondary structural element	Residue Number	Holo- TGIF1-HD		$\Delta\omega_{direct}$ (ppm) (δ_{holo}-δ_{apo})	$\Delta\omega_{CEST}$ (ppm) (δ_{minor}-δ_{major})	Deviation of $\Delta\omega_{CEST}$ (ppm)
		δ_H (ppm)	δ_N (ppm)			
α1	K173	9.01	126.60	1.20	1.12	0.008
	E174	9.55	118.31	-0.50	-0.33	0.016
	S175	7.09	114.59	-0.11	-0.14	0.030
	I178	7.04	118.37	0.27	0.25	0.004
	L179	7.15	120.71	0.41	0.44	0.020
	R180	8.83	119.44	-0.06	0.16	0.029
	D181	8.56	120.24	0.04	0.22	0.002
	E185	8.17	118.72	-0.18	-0.28	0.030
L1	R187	6.61	118.42	0.12	0.18	0.058
	Y188	7.67	115.20	0.00	-0.27	0.033
	S193	9.60	121.29	0.29	0.41	0.018
α2	E194	9.16	120.79	0.39	0.45	0.021
	Q195	8.52	118.93	-0.18	0.26	0.019
	E196	7.91	121.67	0.37	0.54	0.016
	A198	7.47	121.18	-0.22	0.18	0.055
	L199	7.87	121.52	0.22	0.42	0.019
	Q203	8.44	116.05	0.15	0.48	0.017
L2	T204	7.91	103.94	-0.16	-0.14	0.050
	S207	9.35	117.86	0.36	0.39	0.017
α3	T208	8.98	116.11	0.61	0.66	0.012
	L209	8.21	123.67	0.77	0.84	0.013
	K229	7.96	120.42	0.12	0.22	0.024
C-	G231	8.15	108.14	-0.17	-0.04	0.025
	K232	8.08	120.22	0.42	0.23	0.014
	D233	8.38	122.19	0.19	-0.20	0.018
	I239	8.14	122.26	-0.44	0.11	0.018
	S240	8.31	118.57	-0.63	-0.45	0.006
	R241	8.35	122.79	-0.41	-0.22	0.020

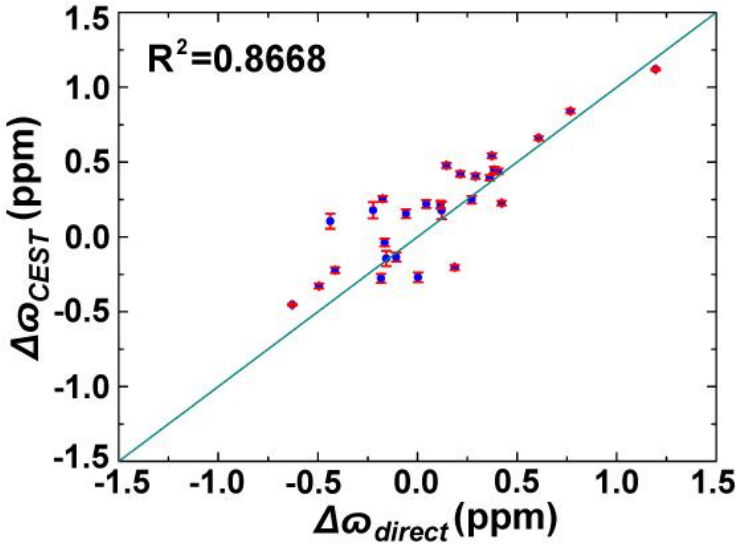

Fig. S1 Correlation between the $\Delta\omega_{direct}$ values detected by ^{1}H-^{15}N HSQC and the $\Delta\omega_{CEST}$ values fitted by CEST shown in Table. S1.

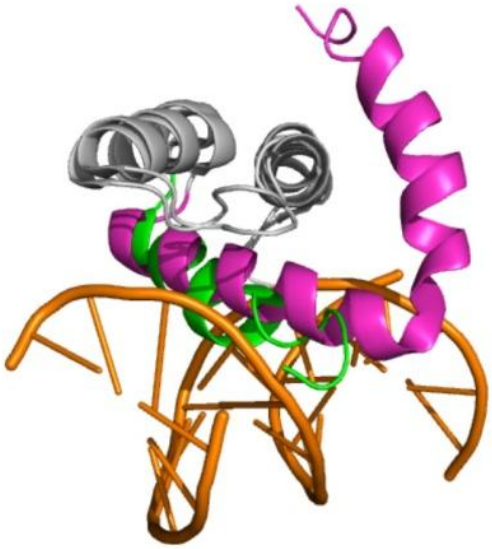

Fig. S2 A structure alignment of free PBX1-HD (green, PDB ID: 1DU6) and PBX1-HD:DNA complex (magenta, PDB ID: 1LFU). The regions with gray color are highly similar with a RMSD of 1.565 Å. The free PBX1-HD structure does not contain the region forming the fourth α-helix in complex structure.

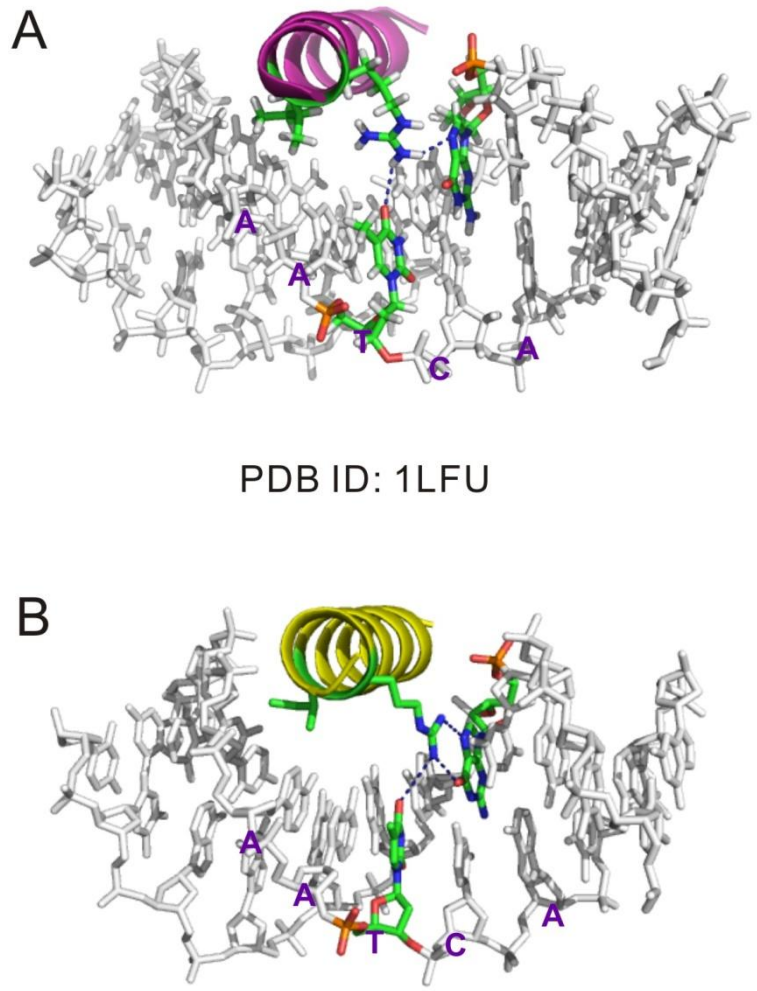

Fig. S3 The roles of I289 and R290 of PBX1 in specific DNA binding. The PBX1-HD:DNA complex structures determined through NMR (A, PDB ID: 1LFU) and X-ray (B, PDB ID: 1B72) are shown with the consensus sequence. Only the α3 helix of PBX1-HD is shown for clarity in either magenta (A) or yellow (B). The side chains of I289 and R290 are displayed, with the hydrogen bonds formed between R290 and two bases (dT and dG) in blue dashed lines.