Supplementary Information for:

Predicting the coordination geometry for Mg^{2+} in p53 DNA-binding domain: Insights from computational studies

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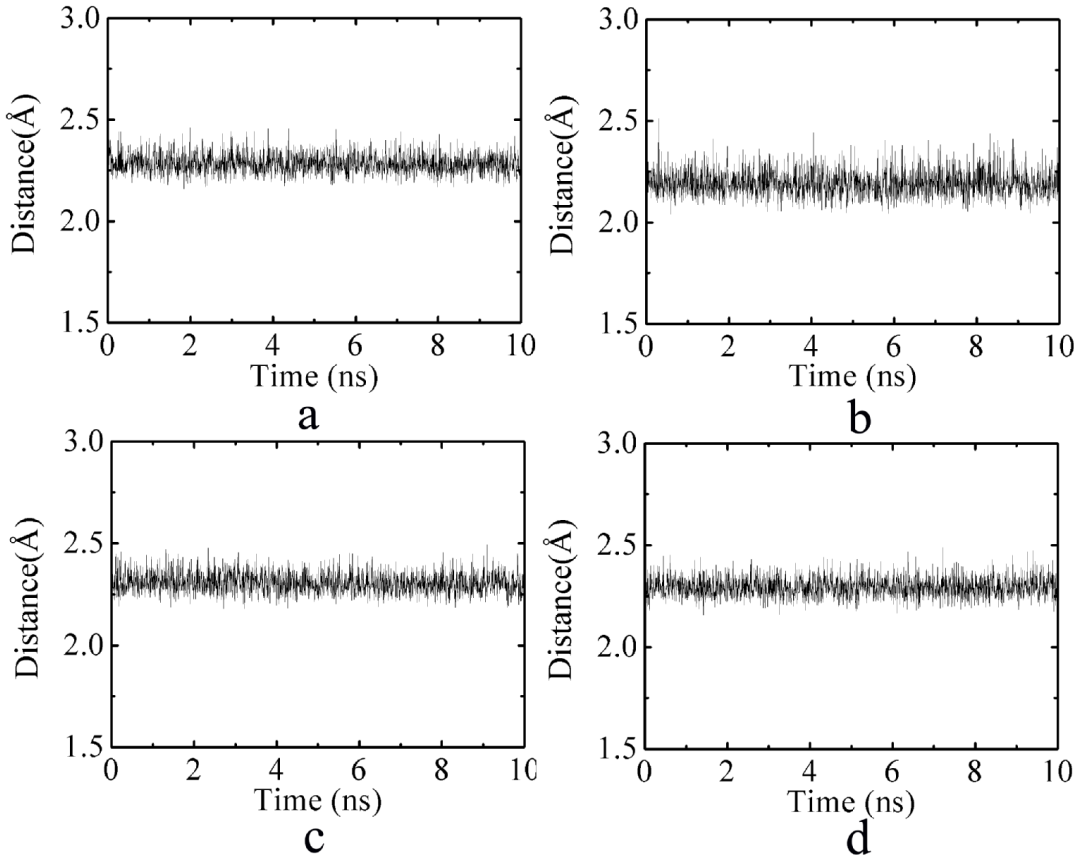
Table S1 The second-order perturbation energies $E(2)$ (kcal mol^{-1}) from NBO

Donor NBO (i)	Acceptor NBO (j)	$E(2)$
	Zn^{2+}·Cys^{-}_3·His	
LP (3) S1	RY*(1)Zn	12.20
LP (3) S1	BD*(1) S2-Zn	17.99
LP (3) S1	BD*(1) S3-Zn	19.24
BD (1) S2-Zn	BD*(1) S3-Zn	31.81
BD (1) S3-Zn	BD*(1) S2-Zn	29.23
	Mg^{2+}·Cys^{-}_3·His	
LP (3) S1	LP*(1)Mg	51.33
LP (1) N	LP*(1)Mg	19.96
LP (3) S2	LP*(1)Mg	52.24
LP (3) S3	LP*(1)Mg	48.43
	Mg^{2+}·Cys^{-}_3·His·W_2-B	
LP (3) S1	LP*(1)Mg	43.36
LP (1) N	LP*(1)Mg	19.05
LP (3) S2	LP*(1)Mg	37.02
LP (2) S3	LP*(1)Mg	18.27
LP (3) S3	LP*(1)Mg	15.85
LP (2) O1	LP*(1)Mg	13.40
LP (2) O2	LP*(1)Mg	12.08

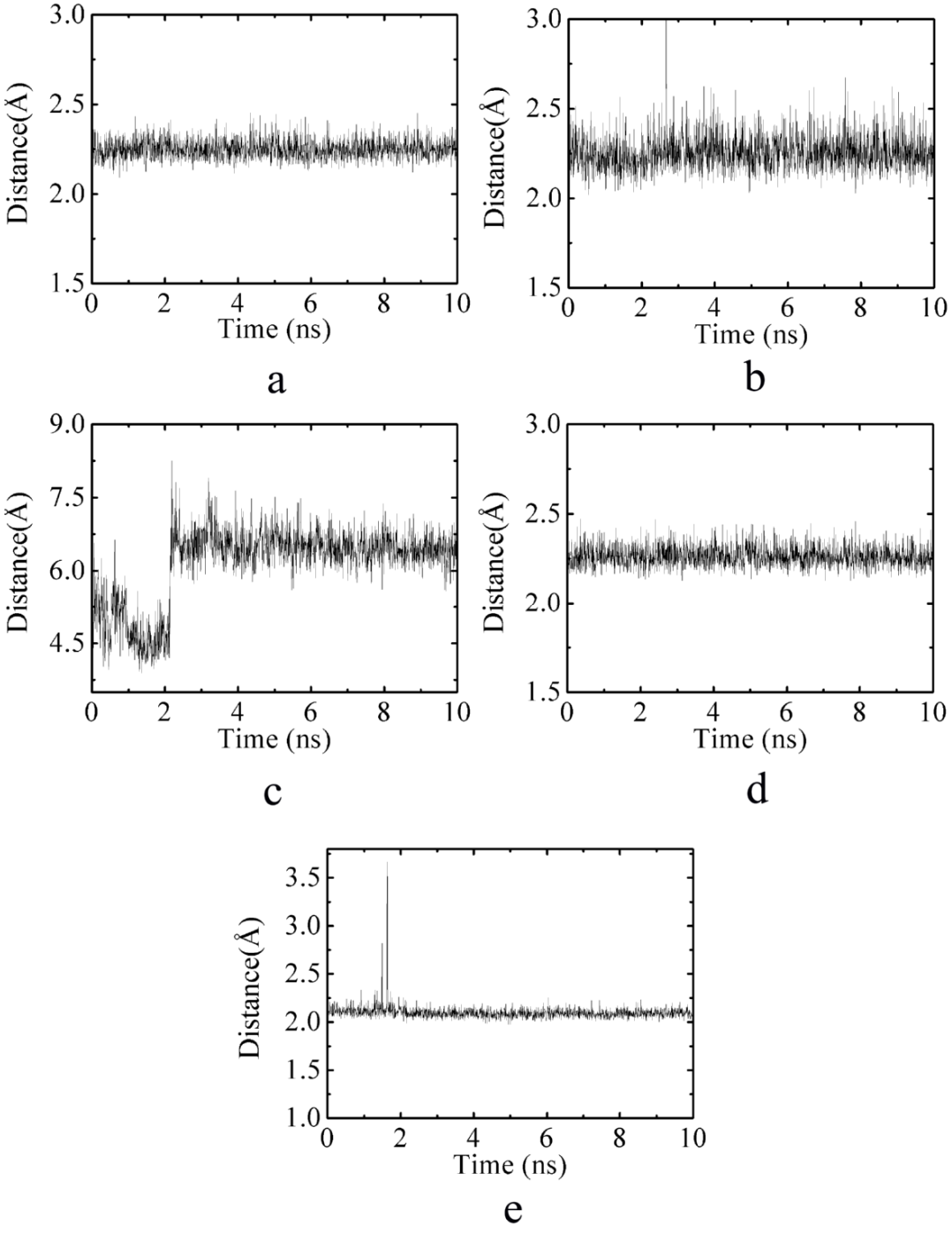
	Mg^{2+}·Cys_3·His	
LP (2) S1	LP*(1)Mg	39.66
LP (1) N	LP*(1)Mg	27.99
LP (2) S2	LP*(1)Mg	41.66
LP (2) S3	LP*(1)Mg	39.91
	Mg^{2+}·Cys_3·His·W_2-B	
LP (2) S1	LP*(1)Mg	30.45
LP (1) N	LP*(1)Mg	25.41
LP (2) S2	LP*(1)Mg	31.96
LP (2) S3	LP*(1)Mg	28.56
LP (2) O2	LP*(1)Mg	17.63
LP (2) O1	LP*(1)Mg	17.98
	Mg^{2+}·Cys_2·His·W_3	
LP (2) S1	LP*(1)Mg	33.39
LP (1) N	LP*(1)Mg	25.30
LP (2) S2	LP*(1)Mg	27.47
LP (2) O3	LP*(1)Mg	18.46
LP (2) O1	LP*(1)Mg	18.91
LP (2) O2	LP*(1)Mg	18.10
	Mg^{2+}·Cys^{-}_2·His·W_3	
LP (2) S1	LP*(1)Mg	10.66
LP (3) S1	LP*(1)Mg	34.83
LP (1) N	LP*(1)Mg	25.47
LP (3) S2	LP*(1)Mg	43.27
LP (2) O3	LP*(1)Mg	14.96
LP (2) O2	LP*(1)Mg	17.16
LP (2) O1	LP*(1)Mg	16.79
	Mg^{2+}·Cys^{-}_2·W_4	
LP (3) S2	LP*(1)Mg	51.66
LP (3) S1	LP*(1)Mg	41.51

LP (2) O1	LP*(1)Mg	18.03
LP (2) O3	LP*(1)Mg	17.93
LP (2) O4	LP*(1)Mg	16.13
LP (2) O2	LP*(1)Mg	16.98
	Mg^{2+}·Cys^{-}·His·W_4	
LP (1) N	LP*(1)Mg	24.85
LP (3) S1	LP*(1)Mg	48.51
LP (2) O4	LP*(1)Mg	19.41
LP (2) O1	LP*(1)Mg	17.05
LP (2) O3	LP*(1)Mg	21.43
LP (2) O2	LP*(1)Mg	18.45
	Mg^{2+}·Cys·Cys^{-}·His·W_3	
LP (2) S1	LP*(1)Mg	27.89
LP (1) N	LP*(1)Mg	24.81
LP (3) S2	LP*(1)Mg	47.75
LP (2) O3	LP*(1)Mg	17.25
LP (2) O2	LP*(1)Mg	17.80
LP (2) O1	LP*(1)Mg	18.44
	Mg^{2+}·Cys_2·Cys^{-}·His	
LP (2) S1	LP*(1)Mg	34.48
LP (1) N	LP*(1)Mg	26.29
LP (2) S2	LP*(1)Mg	33.43
LP (3) S3	LP*(1)Mg	72.24
	Mg^{2+}·Cys_2·Cys^{-}·His·W_2	
LP (2) S1	LP*(1)Mg	28.40
LP (1) N	LP*(1)Mg	24.14
LP (2) S2	LP*(1)Mg	28.42
LP (3) S3	LP*(1)Mg	44.91
LP (2) O1	LP*(1)Mg	15.66
LP (2) O2	LP*(1)Mg	16.36

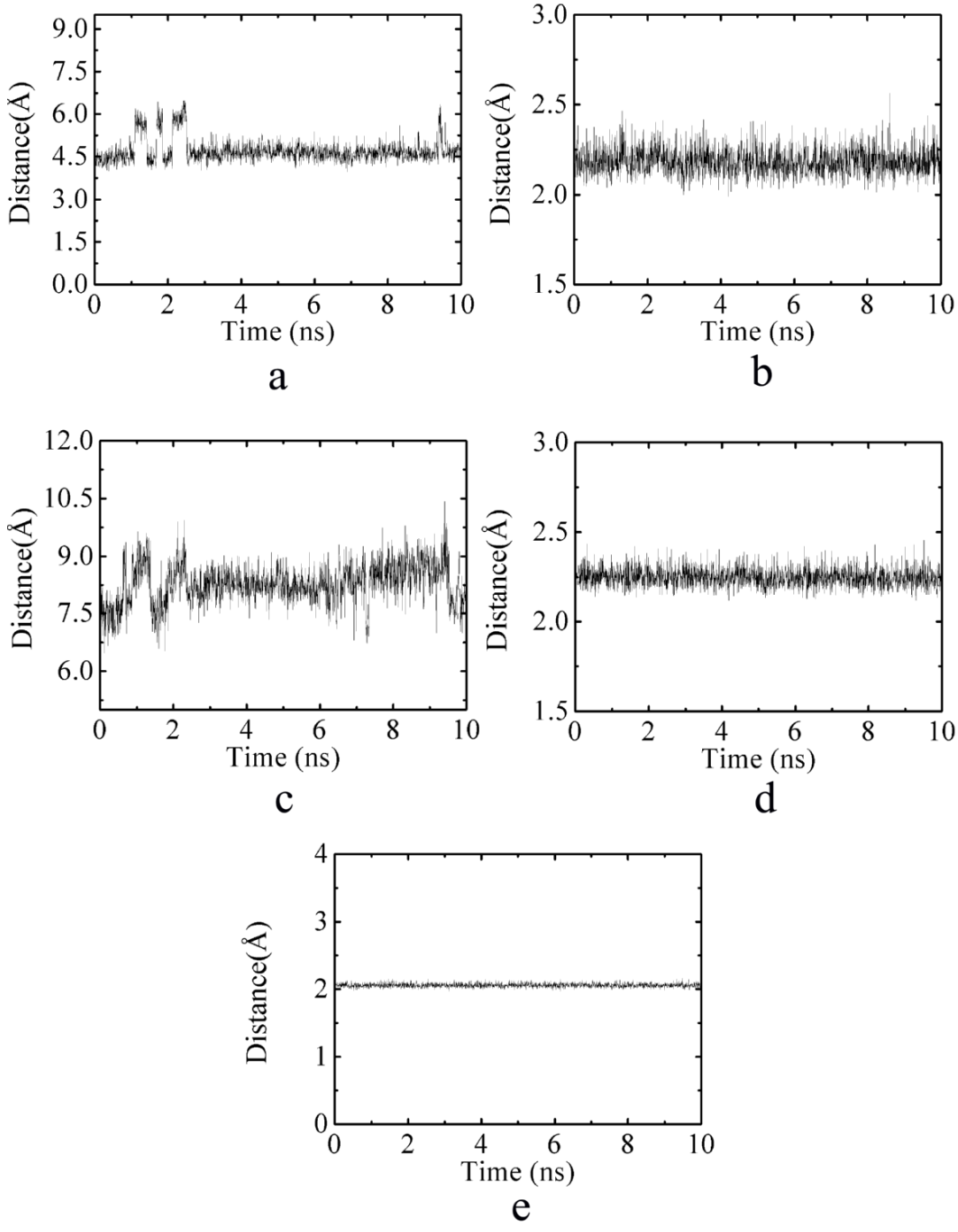
BD denotes bonding orbital; BD* denotes antibonding orbital; LP denotes lone pair; LP* denotes unoccupied orbital. For LP, (1), (2) and (3) denote the first, the second and the third lone pair electron, respectively. RY* denotes Rydberg orbital.



A



B



C

Fig. S1 (a) Time evolution of the distance between the metal ion and the S_γ atom of Cys176.
(b) Time evolution of the distance between the metal ion and the $N_{\delta 1}$ atom of His179.
(c) Time evolution of the distance between the metal ion and the S_γ atom of Cys238.
(d) Time evolution of the distance between the metal ion and the S_γ atom of Cys242.
(e) Time evolution of the average distance between the metal ion and the oxygen atoms of water molecules.
(A) Zn^{2+}-p53DBD. (B) Mg^{2+}-p53DBD (1H). (C) Mg^{2+}-p53DBD (2H).

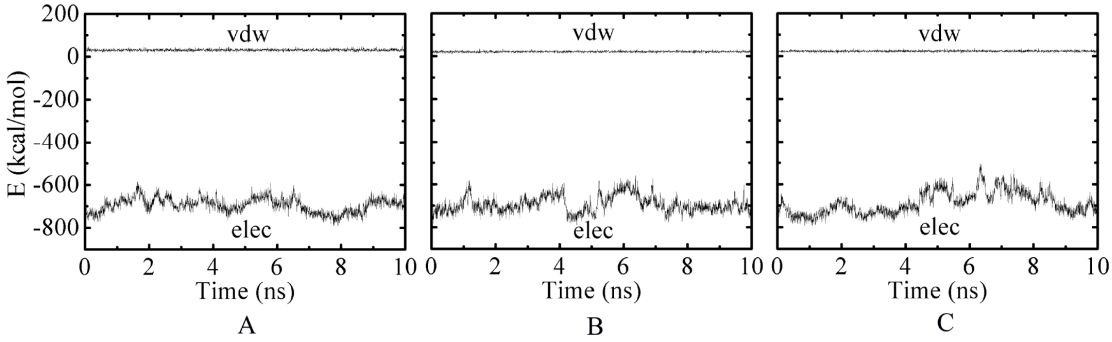


Fig. S2 Interaction energy between the metal ion and all the other atoms (protein and water) in (A) Zn^{2+}-p53DBD. (B) Mg^{2+}-p53DBD (1H). (C) Mg^{2+}-p53DBD (2H).