

Supporting Information

For

Structure-guided Development of Pb²⁺-binding DNA Aptamers

Hehua Liu^{1,+}, Yanqing Gao^{1,+}, Johnsi Mathivanan^{2,+}, Fusheng Shen², Xi Chen¹,
Yangyang Li¹, Zhiwei Shao¹, Yixi Zhang¹, Qiyuan Shao¹, Jia Sheng^{2,*}, Jianhua Gan^{1,*}

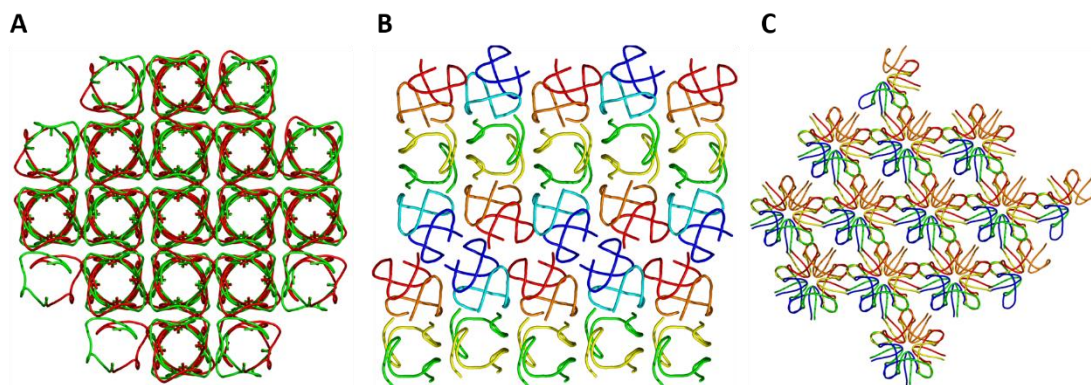


Fig. S1: Packing of (A) A-form TBA-Pb²⁺ complex, (B) B-form TBA-Pb²⁺ complex and (C) G8C-Pb²⁺ complex in the crystal lattice. Figures were displayed using PyMOL (<http://www.pymol.org/>).

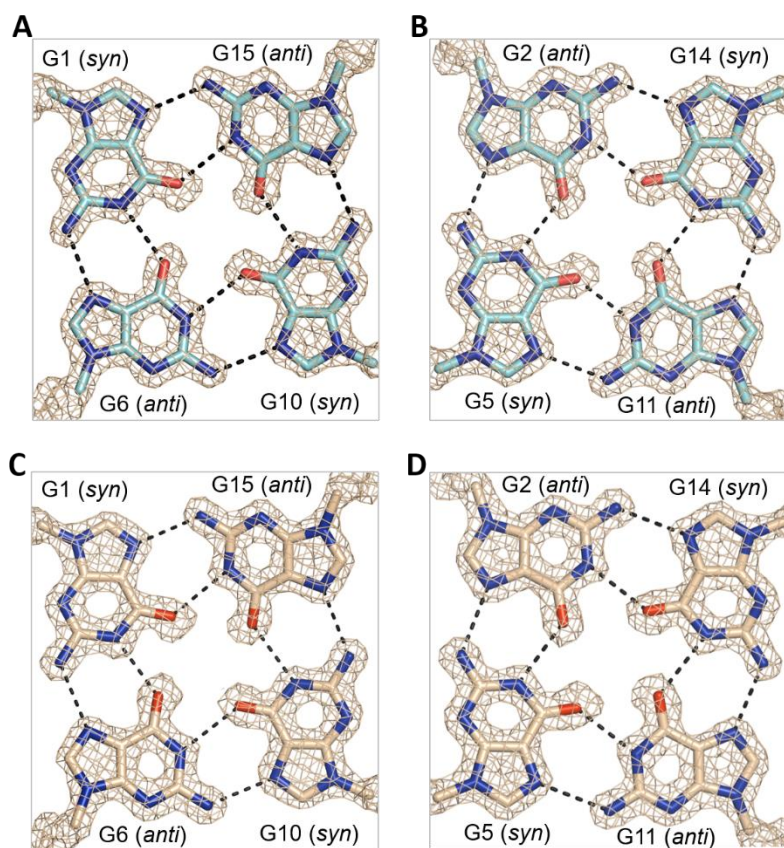


Fig. S2: G-tetrads observed in the A-form TBA-Pb²⁺ complex structure. (A-B) G-tetrads formed by TBA molecule A. (C-D) G-tetrads formed by TBA molecule B. Nucleobases of the G-tetrads are shown as sticks outlined with 2F_o-F_c electron density maps (contoured at 1.5 σ level). The N1-O6 and N2-N7 H-bond interactions are indicated by black dashed lines. Figures were displayed using PyMOL (<http://www.pymol.org/>).

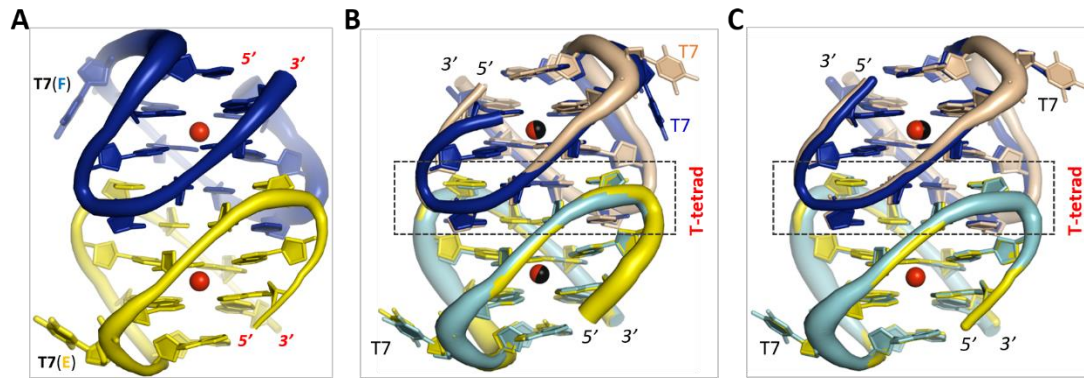


Fig. S3: Comparison of the A- and B-form TBA-Pb²⁺ structure. (A) Overall folding of the EF dimer of the B-form structure. (B) Superposition of the AB dimer of the B-form structure with the A-form structure. (C) Superposition of the CD dimer of the B-form structure with the A-form structure. All dimers of the B-form structure are colored in yellow and blue. The A-form structure is colored in cyan and wheat in panels (B) and (C). Figures were displayed using PyMOL (<http://www.pymol.org/>).

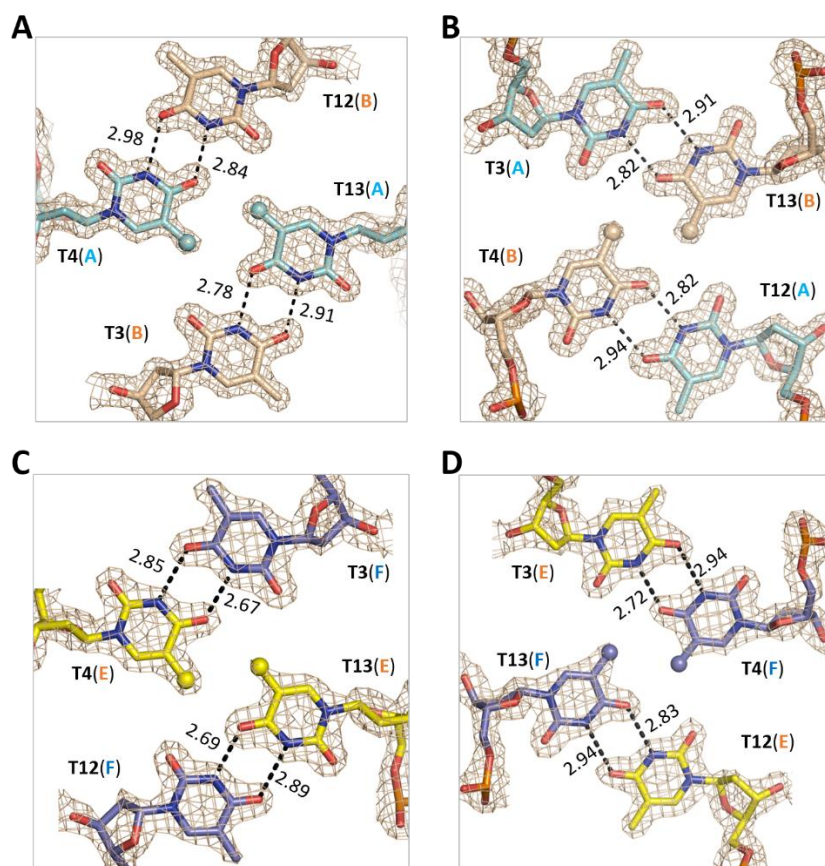


Fig. S4: Interactions formed between the TT linker nucleotides. **(A-B)** Detailed H-bond interactions formed between the T3T4 and T12T13 linkers of the A-form TBA-Pb²⁺ structure. **(C-D)** Detailed H-bond interactions formed between the T3T4 and T12T13 linkers of the EF dimer of the B-form TBA-Pb²⁺ structure. The 5-methyl groups of T4 and T13 are shown as spheres. The $2F_o - F_c$ electron density maps are contoured at 1.5σ level in panels **(A)** and **(B)**, whereas they are contoured at 1.2σ level in panels **(C)** and **(D)**. Figures were displayed using PyMOL (<http://www.pymol.org/>).

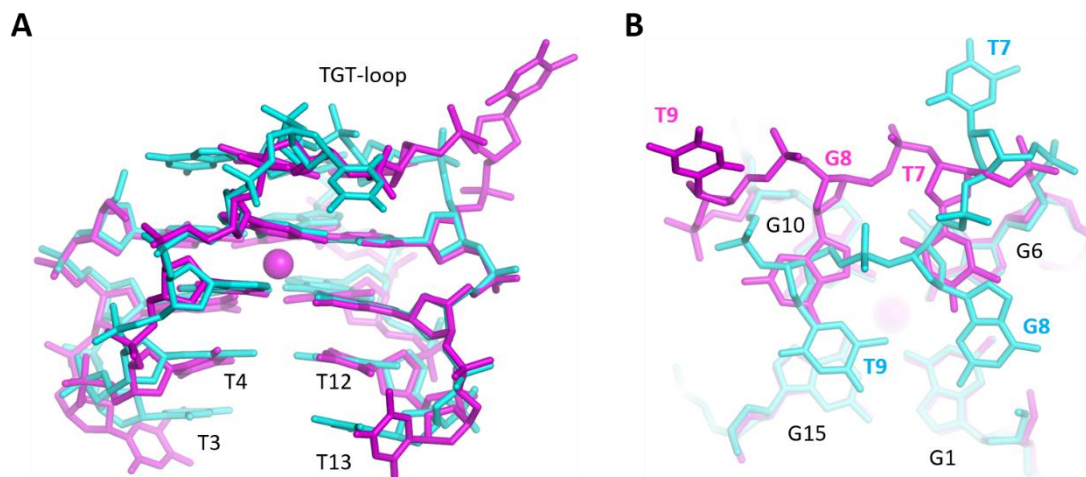


Fig. S5: (A) Superposition of TBA molecules of the A-form TBA-Pb²⁺ complex and the TBA-thrombin complex (PDB_ID: 4DII). (B) Superposition showing the conformational difference of T7G8T9 linkers. The Pb²⁺-complexed TBA molecule is shown as sticks in cyan. TBA and K⁺ observed in the TBA-thrombin complex are shown as magenta sticks and sphere, respectively. Figures were displayed using PyMOL (<http://www.pymol.org/>).

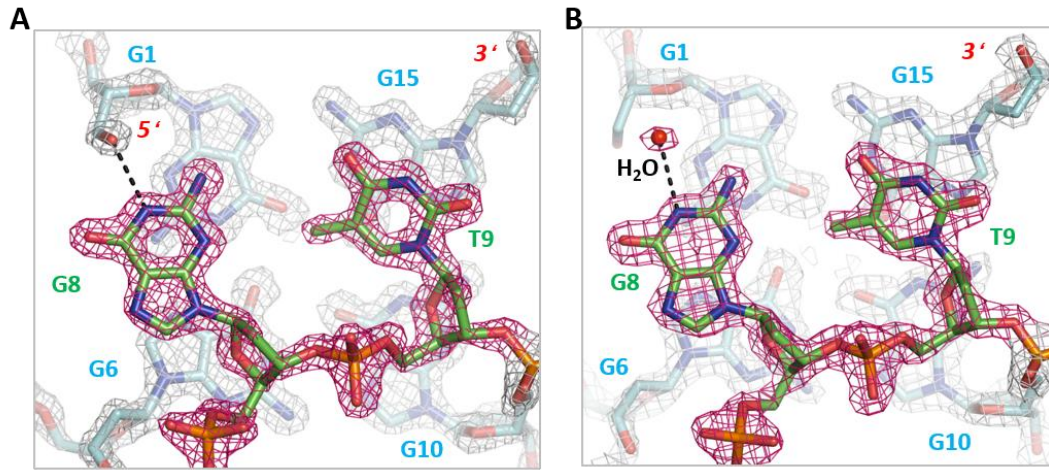


Fig. S6: Conformation and interaction of G8 in (A) the A-form and (B) the B-form complex structures. G8, T9 and nucleotides of the G-tetrad are shown as sticks. Water molecules are shown as red spheres. The $2F_o-F_c$ electron density maps are all contoured at 1.5σ level.