NMR structure of human telomeric RNA (TERRA): Stacking of two G-quadruplex blocks in K^+ solution

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SUPPORTING INFORMATION

SUPPLEMENTARY FIGURES

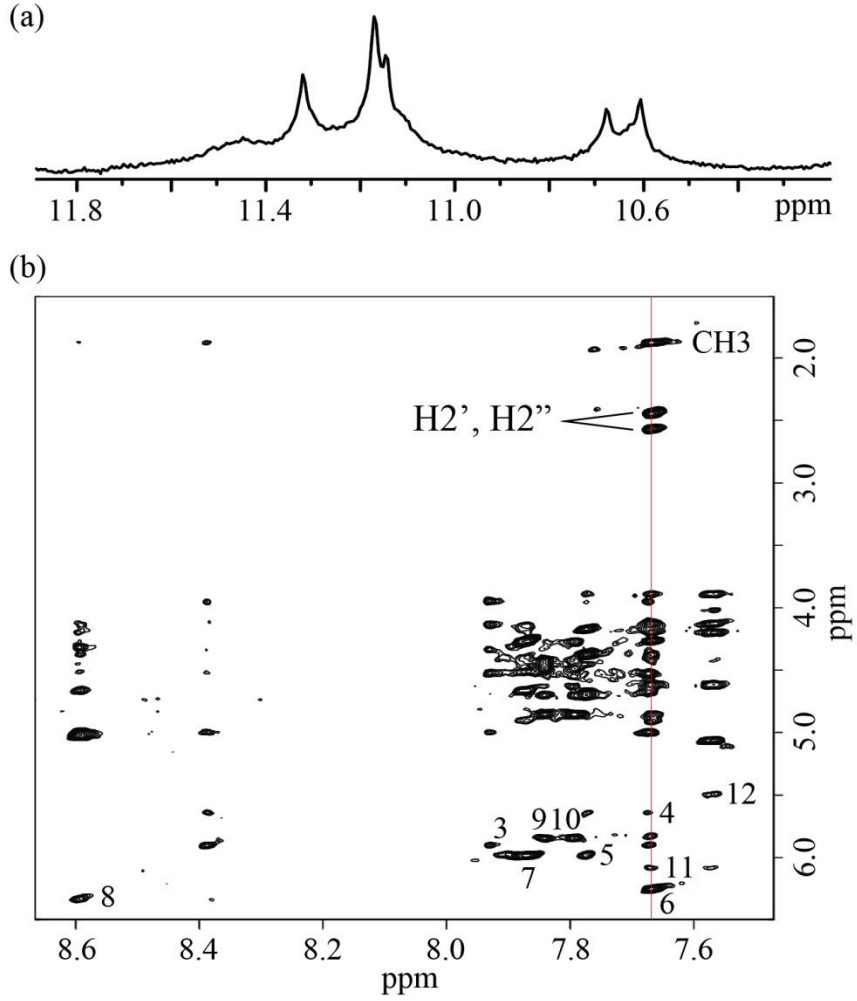

Figure S1. (a) Imino proton spectrum and (b) NOESY spectrum of the site-specific ribose-to-deoxyribose substituted sequence (dT6), r(GGG) **dT** r(UAGGGU), in K^+ solution. Vertical lines are drawn on the frequency of the dT6(H6) proton. The up-field shift of the H2'/H2" chemical shifts for the substituted base is indicated. Intra-residue H6/H8-H1' cross-peaks are labelled with residues number.

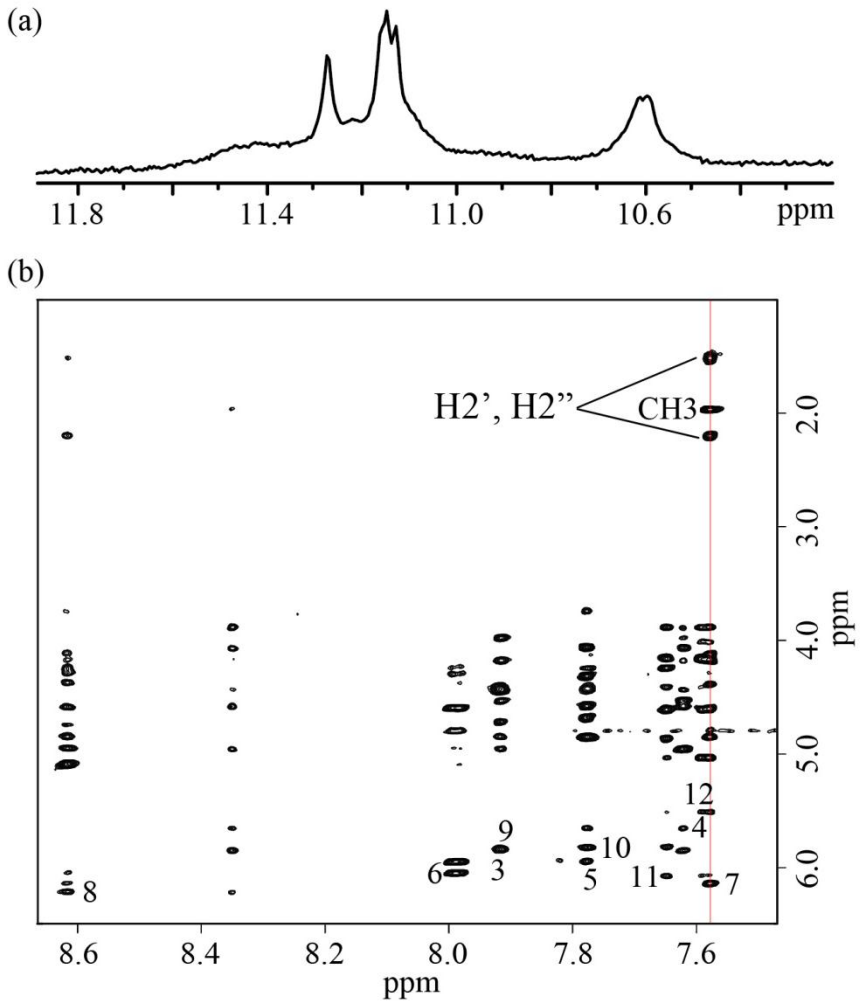

Figure S2. (a) Imino proton spectrum and (b) NOESY spectrum of the site-specific ribose-to-deoxyribose substituted sequence (dT7), r(GGGU) **dT** r(AGGGU), in K^+ solution. Vertical lines are drawn on the frequency of the dT7(H6) proton. The up-field shift of the H2'/H2" chemical shifts for the substituted base is indicated. Intra-residue H6/H8-H1' cross-peaks are labelled with residues number.

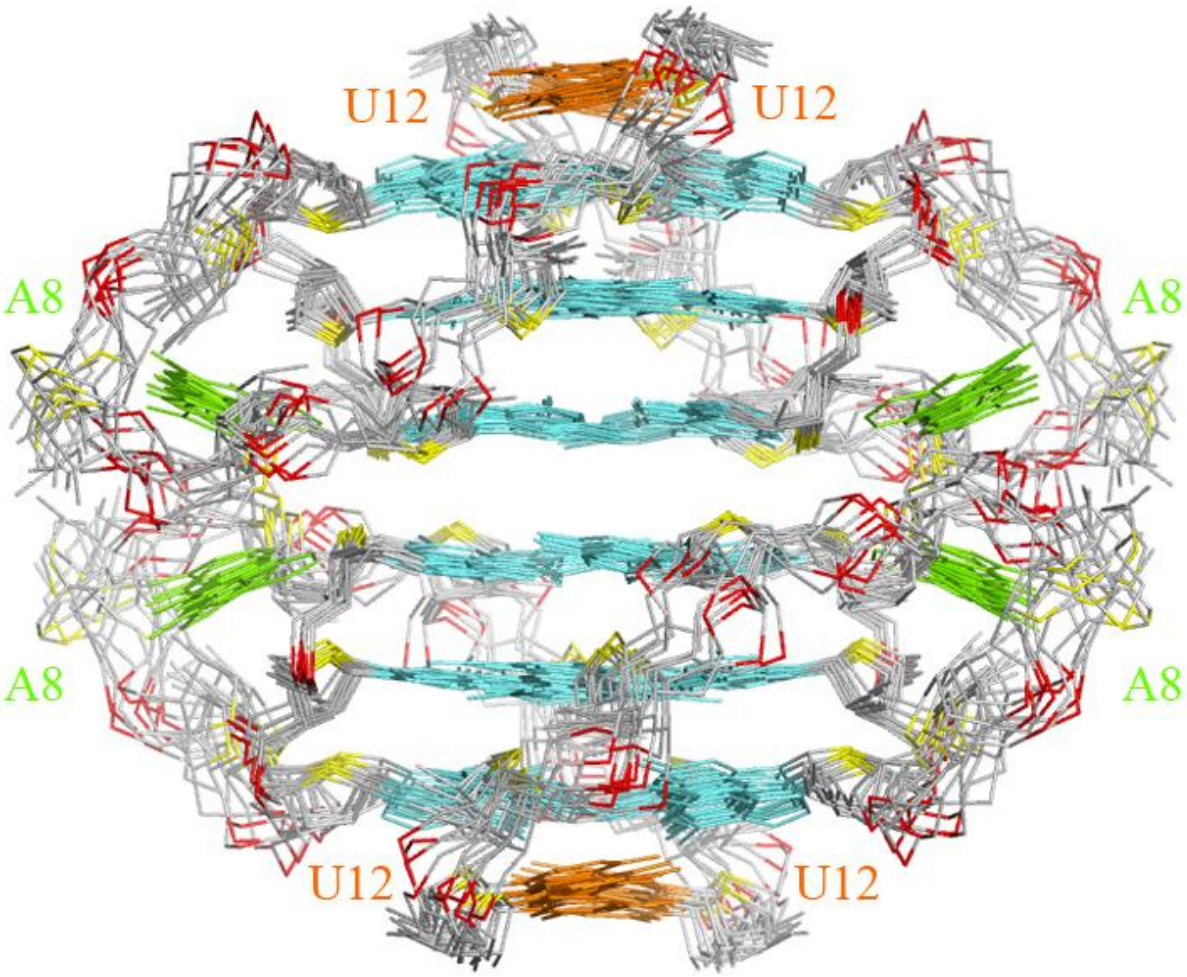

Figure S3. Superposition of ten lowest-energy computed G-quadruplex structures formed by the 10-nt human TERRA sequence r(GGGUUAGGGU) in K^+ solution. NOE restraints in Table 3 were omitted during the calculation. The bases of U6 and U7 are not displayed for clarity. Bases of guanines are colored cyan; adenines, green; uracils, orange; backbone, grey; O4' atoms, yellow; P atoms, red.

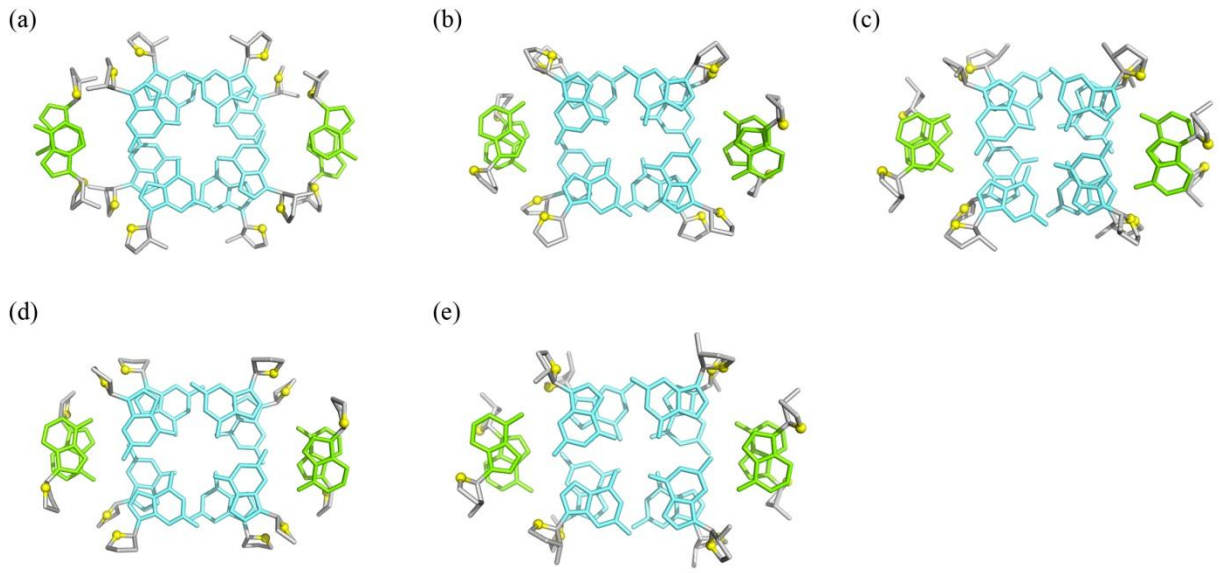

Figure S4. Top view of the A:(G:G:G:G):A hexad stacking interfaces of G-quadruplexes formed by (a) the 10-nt human TERRA sequence r(UAGGGUUAGGGU) in K^+ solution reported here; (b) $d(GGA)_2$ in Na^+ solution (PDB ID: 1EEG); (c) r(GGAUUUUGGA) in K^+ solution (PDB ID: 1MY9); (d) d(TAGGGTTAGGGT) co-crystallized with naphthalene diimide ligand (PDB ID: 3CCO); (e) $r(GGA)_4$ in K^+ solution (PDB ID: 2RQJ). Bases of guanines are colored cyan; adenines, green; sugars, grey; O4' atoms, yellow.

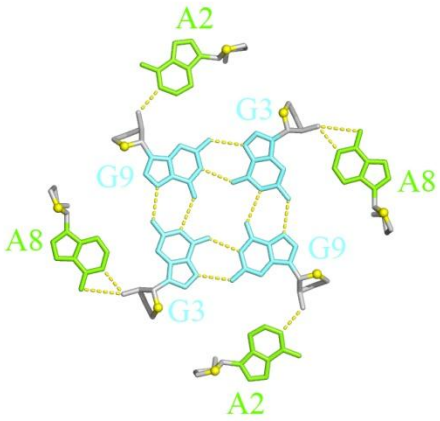

Figure S5. Stacking interface in the crystal structure of the 12-nt human TERRA sequence r(UAGGGUUAGGGU) bound to acridine (PDB ID: 3MIJ). Bases of guanines are colored cyan; adenines, green; sugars, grey; O4' atoms, yellow. Hydrogen bonds are indicated by yellow dash lines.