

**Figure S4.** Selected fragments of 10-30 ns averaged MD structures of wild-type (a, c, e) and mutant hCG: (b) p.V56L, (d) p.P73R, (f) p.R8W. Hydrogen bonds are shown as dotted lines, positions under study are highlighted in red. Residues of hCG  $\alpha$ -subunit are denoted with '.A' and residues of the  $\beta$ -subunit with '.B'. Only some residues are displayed to avoid cluttering.

