

**Fig. 4.** (a) Detail of the crystal packing of **1**. (b,c) Theoretical models used to evaluate the interaction energies. Distances in Å. (d) NCI surface of the assembly present in compound **1**. The gradient cut-off is s = 0.35 a.u., and the color scale is −0.04 <*ρ*< 0.04 a.u.