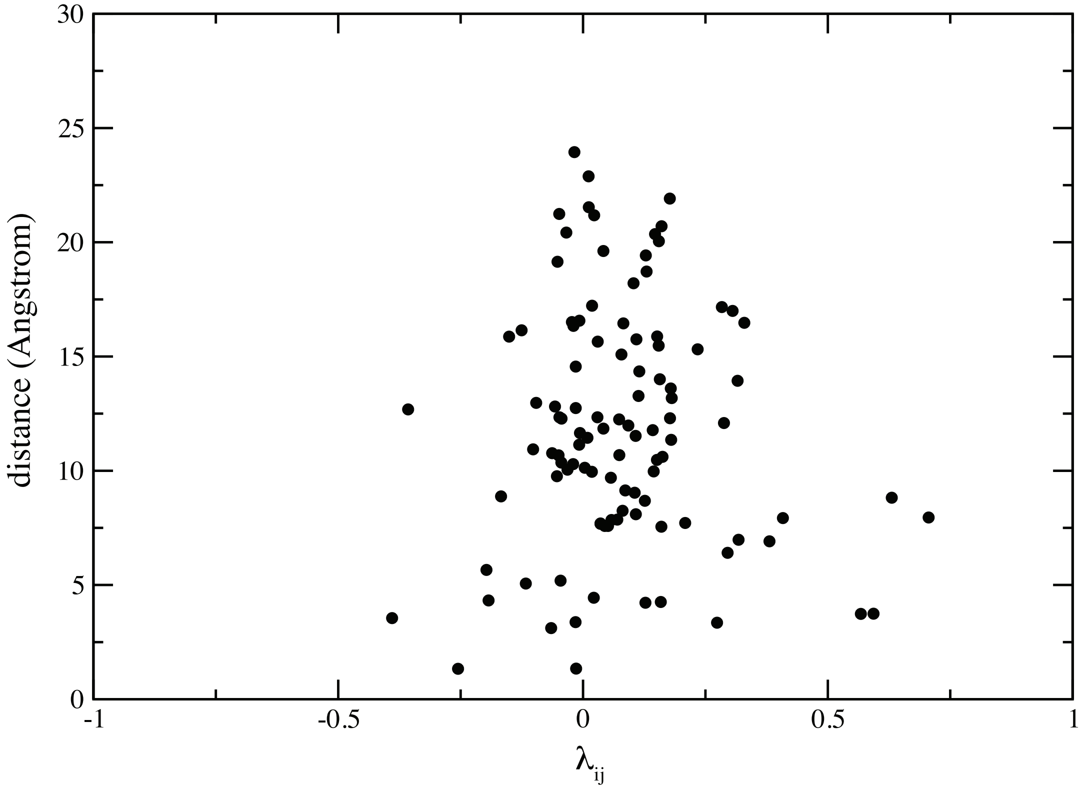

Additional File 3: Scatterplot of distance vs λ_{ij} parameters estimated using I and J values of ±1 as described in the Methods for the 15-residue group 10–20–33–36–46–54–55–63–71–73–74–82–84–90–93 in the PI2+ cohort. The value along the y-axis is the closest distance between any two heavy atoms of the two residues based on the crystal structure of wild type protease (PDB ID 1PRO).