Megestrol acetate is a synthetic derivative of naturally occurring steroid hormone progesterone [1]. It crystallizes in P21 space group with two molecules in the asymmetric unit. The X-ray diffraction intensity data of megestrol acetate crystal has been collected at low temperature 110 K. The crystal and molecular structure was determined and the geometry of both molecules was studied. The conformations of two megestrol acetate molecules are largely differ in the D-ring and the two bulky groups. The Hirshfeld surface and finger print plot insights the strength of the intermolecular interactions [2]. The molecular packing in the crystal is stabilized by the weak and strong C–H···O intermolecular interactions. Further, a theoretical charge density analysis of megestrol acetate molecules has been performed to understand its bond topological and electrostatic properties using density functional theory calculations coupled with quantum theory of atoms in molecules (QTAIM) [3]. The charge density distribution of megestrol acetate allows to distinguish the charge density of various bonds. The electrostatic potential shows the high electropositive and electronegative regions of the molecules. The global reactivity descriptors elucidate the chemical and physical properties of the megestrol acetate molecule.


Keywords: Hirshfeld Surface, Electron density, Delocalization index