Prednisolone acetate is an ophthalmic drug that belongs to a class of corticosteroids [1]. The chemical properties of the molecule rest on the Charge–density distribution [2]. A thorough information about planarity, structural parameters, stereochemistry and shared arrangement of the molecule is necessary for the understanding of structure–property relationship. The structure was refined using the classical independent atom model (IAM) and a transferred multipolar atom model using the ELMAM2 database [3]. The results from the two refinements have been compared. The ELMAM2 refinement has been found to be superior in terms of the refinement statistics. It has been shown that certain electron-density-derived properties can be calculated on the basis of the transferred parameters for crystals which diffract to ordinary resolution. This procedure better leads to complete understanding of mechanism of drug action Figure 1.

Figure 1 : A three-dimensional electron-density isosurface generated at an electron-density value of 0.05 eÅ³, coloured according to the electrostatic potential.


Keywords: Crystal structure, ELMAM2, Prednisolone acetate