Prostate cancer is now the most common malignancy and the second leading cause of cancer death in North American males. Androgen antagonists offer a potentially useful treatment for androgen-mediated diseases, such as: prostate cancer, hirsutism, acne, seborrhea, androgenic alopecia and benign prostatic hyperplasia. Although surgery presently represents usual treatment for prostatic cancer, there are also several other alternative modalities currently available for treatment of these androgen-dependent afflictions. At the present time, the most common therapy for treating prostate cancer and benign prostatic hyperplasia is blockage of the androgen receptor by androgen antagonists, or inhibition of the conversion of testosterone to the more active androgen dihydrotestosterone by the enzyme 5α-reductase.

In this paper, we describe the synthesis and an X-ray structure determination of 3β-benzoyloxy-4-pregnen-16α,17α-epoxy-6,20-dione 7. The preparation of 7 is described in Scheme 1.

X-ray data for crystals of the title compound were collected by graphite-monochromatized Mo Kα radiation at 293 K. No absorption correction was applied. The structure was solved by direct methods and refined by full-matrix least squares with anisotropic temperature factors for the non-hydrogen atoms. The positions of all H atoms were calculated geometrically, and a riding model was used in their refinement, with the C–H distances in the range of 0.85–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The software used to prepare material for publication was PARS97. Table 1 summarizes the crystal and experimental data. The molecular structure is shown in Fig. 1. The bond angles, the final atomic parameters for the hydrogen atoms, the anisotropic thermal parameters for non-hydrogen atoms, and the observed and calculated structure factors may be obtained from the first author.

The molecule consists of three six-membered rings and one

![Scheme 1](image1)

![Fig. 1](image2)
For the puckering-parameter values ($\phi_2$, $\theta_2$ and $Q$), the six-membered rings A, B and C occur in envelope (1E), distorted chair (1$C_4$) and distorted chair (1$C_4$) conformations, respectively. Ring D occurs in a distorted-envelope conformation. The bond lengths and angles are normal. The absolute configuration is inferred from the known stereochemistry of 3$\beta$-acetoxypregna-5,16-diene-20-one \(^{1}\). Compound 1 is commercially available. The stereochemistry of the title compound is as follows: C8 – $\beta$H is trans to C9 – $\alpha$H; C8 – $\beta$H is trans to C14 – $\alpha$H; C9 – $\alpha$H is trans to C10 – $\beta$CH$_3$; C13 – $\beta$CH$_3$ is trans to C14. There are four intramolecular C – H···O interactions [C3···O2, C4···O4, C19···O3, C21···O5 2.689(3), 2.786(3), 3.073(3), 2.895(3)Å; H3···O2, H4···O4, H19C···O3, H21A···O5 2.331(2), 2.457(2), 2.530(2), 2.434(2)Å; C3 – H3···O2, C4 – H4···O4, C19 – H19C···O3, C21 – H21A···O5 100.6(1), 100.9(2), 115.9(1), 109.2(2)˚]. In addition, there are three intermolecular C – H···O interactions <3.4 Å: C21···O2 ($x$, +$y$, +$z$); C18···O4 ($-x$, +$y$, +$z$); C21···O2 (+$x$, +$y$, +$z$) 3.387(3), 3.389(3) and 3.274(3)Å, respectively. Apart from the C···O intra- and intermolecular contacts, the packing in the crystal is entirely due to van der Waals forces.

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References