

Fig. 1. ORTEP (Johnson, 1965) thermal-ellipsoid (20%) plot, showing atomic labelling. Hydrogens omitted.

nucleus taken from Alzari, Ronco, Rivero & Punte (1986), refined by full-matrix least squares based on F^2 's, weighting scheme $w = 1/[\sigma^2(F) + 0.00344F^2]$, H atoms (parameters not refined) positioned from ΔF synthesis when possible, the others being stereochemically determined, with isotropic thermal parameters as those of bonded C atoms. Isotropic secondary extinction of the form $F' = F(1 - CF^2/\sin\theta)$, applied on F_c , refined value of $C = 1.82 \times 10^{-7}$. Final agreement factors $R = 0.050$, $wR = 0.054$ for 208 parameters refined, max. and min. heights in final difference map: 0.21 and -0.18 e \AA^{-3} , $(\Delta/\sigma)_{\text{max}} = 0.06$. Scattering factors from *International Tables for X-ray Crystallography* (1974), computer program used for refinement: *SHELX76* (Sheldrick, 1976).

Fractional atomic coordinates and equivalent isotropic thermal parameters for non-hydrogen atoms are presented in Table 1; * bond lengths and angles are

* Lists of observed and calculated structure factors, anisotropic thermal parameters for non-hydrogen atoms, positional and isotropic thermal parameters for hydrogen atoms and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44893 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

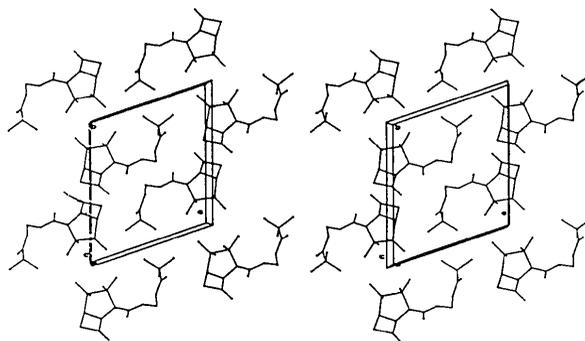


Fig. 2. Stereoview of the molecular packing along c .

listed in Table 2. Atom labelling is shown in Fig. 1; packing diagram in Fig. 2.

Related literature. This work is part of a systematic study on the influence of 1,6-substituents on the conformation of the molecular nucleus of penam derivatives (Punte, Rivero & Alzari, 1986, and references therein).

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