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

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

nucleus taken from Alzari, Ronco, Rivero & Punte (1986), refined by full-matrix least squares based on F'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 Å^{-3}, $(\Delta/\sigma)_{max} = 0.06$. Scattering factors from *International Tables for X-ray Crystallography* (1974), computer program used for refinement: *SHELX*76 (Sheldrick, 1976).

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

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).

---

* 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.
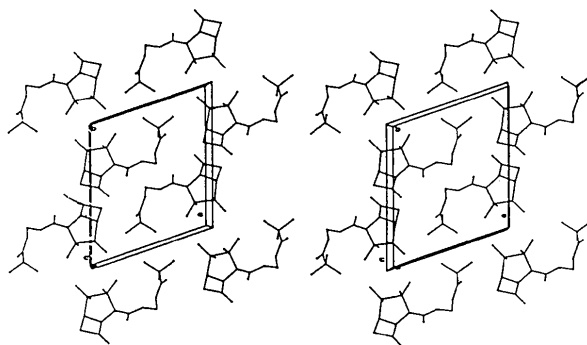
References

ALZARI, P. M., RONCO, A. E., RIVERO, B. E. & PUNTE, G. (1986). *Acta Cryst.* C42, 1032–1034.
EGERT, E. & SHELDRICK, G. M. (1985). *PATSEE*. Fragment search by integrated Patterson and direct methods. Univ. of Göttingen, Federal Republic of Germany.
HAMILTON, W. C. (1959). *Acta Cryst.* 12, 609–610.
International Tables for X-ray Crystallography (1974). Vol. IV, pp. 99–149. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
JOHNSON, C. K. (1965) *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
PUNTE, G., RIVERO, B. E. & ALZARI, P. M. (1986). *Acta Cryst.* C42, 1037–1038.
SHELDRICK, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

International Union of Crystallography

Acta Cryst. (1988). C44, 1328

Microfiche Version of *Acta Crystallographica* and *Journal of Applied Crystallography*

All back volumes of both journals are now available on microfiche, including Volumes 2 and 3 of *Acta*

Crystallographica which have been out of print for many years.

Orders may be placed direct with the publisher (Munksgaard International Publishers Ltd, 35 Nørre Søgade, PO Box 2148, DK-1016 Copenhagen K, Denmark) or with Polycrystal Book Service, from whom prices may also be obtained.