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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.091
Data-to-parameter ratio = 13.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Diphenylmethyl 3-azido-1,1-dioxocephalosporanate

The title compound, $C_{21}H_{20}N_4O_5S$, crystallizes with two molecules in the asymmetric unit. The crystal structure is stabilized by a network of C—H···O hydrogen bonds.

Comment

Tazobactam is a widely used beta-lactamase inhibitor (Bai *et al.*, 2001, Micetich *et al.*, 1987). The title compound, (I), is a by-product of the synthesis of tazobactam and the structure of its benzene solvate has been reported (Liu, 2006). The unsolvated material, (I), was obtained from 6-aminopenicillanic acid, and its structure is reported here (Figs. 1 and 2).

(I)
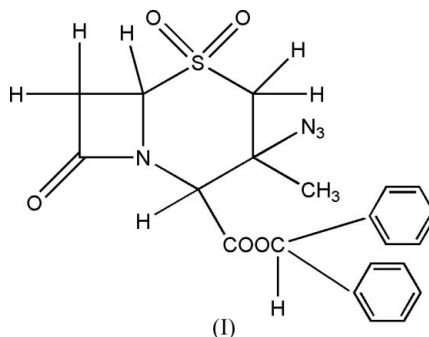
Compound (I) crystallizes with two independent, but structurally quite similar, molecules in the asymmetric unit. All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and similar to those reported for the solvated material (Liu, 2006). The four-membered azetedinone rings are planar (r.m.s. deviations 0.0246 and 0.0249 Å). The thiazine rings adopt chair conformations. The C1/O1/O2/C14/C15 and C22/O6/O7/C35/C36 carboxylate units are also planar (r.m.s. deviations 0.0232 and 0.0383 Å, respectively) and lie approximately orthogonal to the respective thiazine rings. The crystal structure is stabilized by a network of intermolecular C—H···O hydrogen bonds (Fig. 3 and Table 1).

Experimental

The title compound was prepared by the procedure of Bai *et al.* (2001). Colourless single crystals of (I) were grown by slow evaporation of a methanol solution.

Crystal data

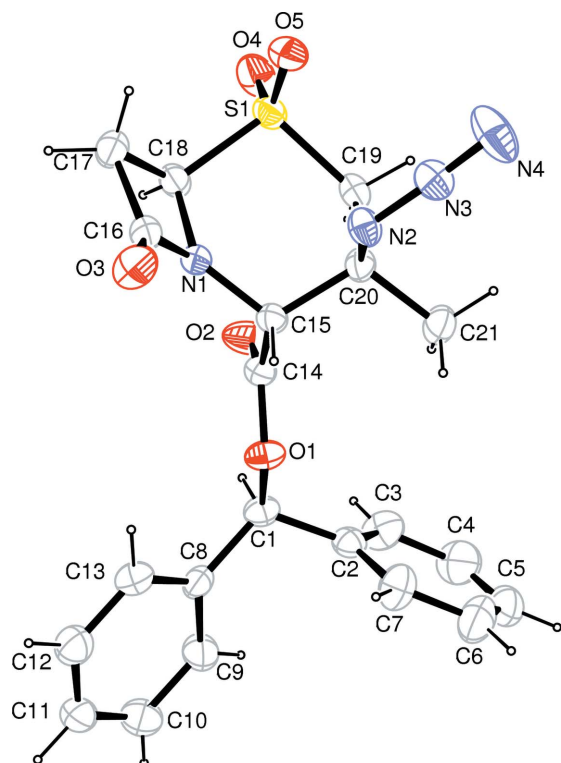|	
$C_{21}H_{20}N_4O_5S$	$Z = 8$
$M_r = 440.47$	$D_x = 1.375$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 10.9030\ (13)$ Å	$\mu = 0.19$ mm^{-1}
$b = 11.3796\ (14)$ Å	$T = 294\ (2)$ K
$c = 34.293\ (4)$ Å	Block, colourless
$V = 4254.8\ (9)$ Å^3	$0.24 \times 0.22 \times 0.18$ mm

Figure 1
One of the two molecules (molecule 1) in the asymmetric unit of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

Figure 3
Packing diagram for (I), with hydrogen bonds drawn as dashed lines.

Data collection

Bruker SMART-1000 CCD area-detector diffractometer	20301 measured reflections
φ and ω scans	7497 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	5529 reflections with $I > 2\sigma(I)$
$T_{min} = 0.943$, $T_{max} = 0.966$	$R_{int} = 0.037$
	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.1929P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
7497 reflections	$\Delta\rho_{min} = -0.25$ e Å^{-3}
561 parameters	Absolute structure: Flack (1983), 2607 Friedel pairs
H-atom parameters constrained	Flack parameter: 0.04 (6)

Table 1
Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C19—H19B···O3[i]	0.97	2.44	3.364 (3)	160
C31—H31···O9[ii]	0.93	2.57	3.446 (6)	157
C36—H36···O10[iii]	0.98	2.25	3.196 (4)	162
C40—H40B···O8[iv]	0.97	2.29	3.235 (4)	166
C18—H18···O7[ii]	0.98	2.50	3.262 (3)	135

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{5}{2}, -z + 2$; (ii) $x, y + 1, z$; (iii) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (iv) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$.

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and $U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})$ for aromatic, C—H = 0.98 Å and $U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})$ for CH, C—H = 0.97 Å and $U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})$ for CH$_2$, and C—H = 0.96 Å and $U_{iso}(\text{H}) = 1.5U_{eq}(\text{C})$ for CH$_3$ H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.
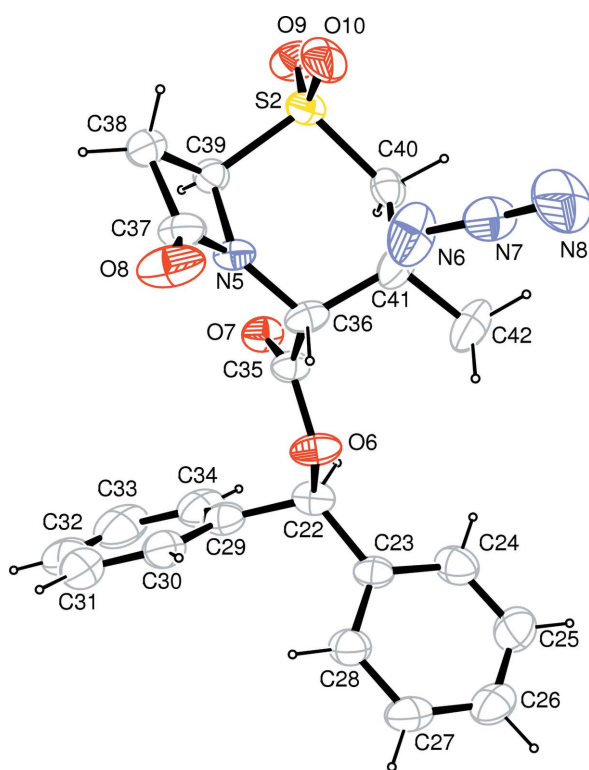
Figure 2
The other molecule (molecule 2) in the asymmetric unit of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.
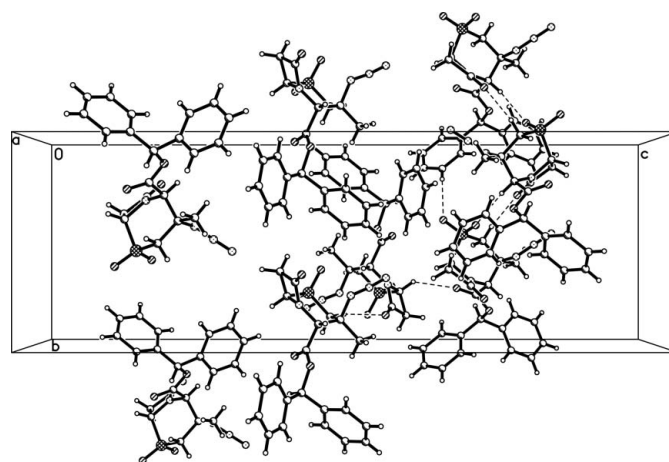
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