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3-Benzoylthymine

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In the title molecule [systematic name: 3-benzoyl-5-methylpyrimidine-2,4(1*H*,3H)-dione], $C_{12}H_{10}N_2O_3$, the dihedral angle between the planes of the two aromatic rings is 83.82 (6)°. In the crystal structure, centrosymmetric dimers are formed *via* intermolecular N—H···O hydrogen bonds (H···O = 1.96 Å).

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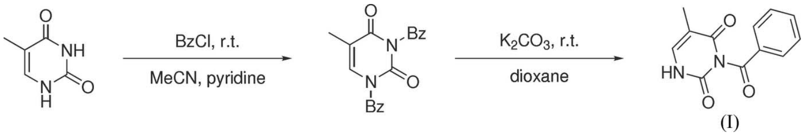
Key indicators

Single-crystal X-ray study
T = 173 K
Mean *σ*(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.123
Data-to-parameter ratio = 15.8

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

Comment

We have investigated the title compound, (I), for potential use in synthesizing hydrogen-bonded architectures for molecular recognition using DNA base pairs.



(I)

The molecular structure of compound (I) is shown in Fig. 1. All bond lengths and angles are within their normal ranges (Allen *et al.*, 1987). The dihedral angle between the two aromatic rings is 83.82 (6)°.

In the crystal structure, centrosymmetric dimers are formed *via* intermolecular N—H···O hydrogen bonds (Table 1).

Experimental

Benzoyl chloride (0.66 ml, 5.67 mmol) was added to a slurry of thymine (0.3249 g, 2.58 mmol) in dry acetonitrile (3 ml) and dry pyridine (1 ml) at room temperature, and stirred for 24 h. The resulting orange solution was evaporated to dryness under reduced pressure. The residue was dissolved in dichloromethane and washed with distilled water, and the organic layer was evaporated to dryness under reduced pressure. The solid was mixed in 1.0 *M* potassium

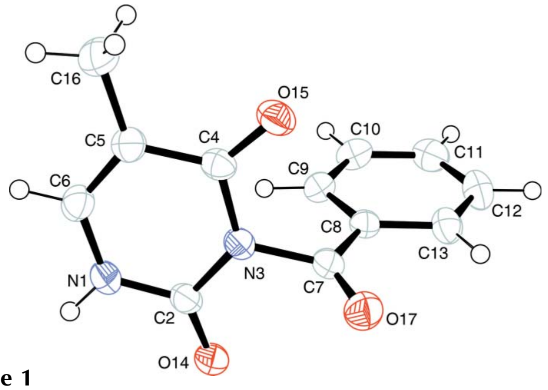


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probabilty level.

carbonate (10 ml) and dioxane (10 ml), sonicated for one minute, and the slurry stirred for 30 min. Glacial acetic acid was added until the pH was 5. The resulting mixture was evaporated under reduced pressure to yield a white solid. The solid was taken up in saturated sodium bicarbonate (10 ml), stirred for 1 h, and washed with distilled water (10 ml). The white solid was then dissolved in acetone (15 ml) and water (15 ml) at room temperature and allowed to stand in an uncapped vial for 18 h to yield colourless needles (yield 0.3206 g, 1.40 mmol, 55%). The identity of the title compound was confirmed by ^{1}H NMR spectroscopy (Frieden *et al.*, 1998).

Crystal data

$C_{12}H_{10}N_2O_3$
$M_r = 230.22$
Orthorhombic, *Pbca*
$a = 8.729$ (2) Å
$b = 9.514$ (2) Å
$c = 25.796$ (5) Å
$V = 2142.3$ (8) Å^3
$Z = 8$
$D_x = 1.428$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 173$ (2) K
Prism, colourless
0.18 × 0.14 × 0.10 mm

Data collection

Nonius KappaCCD area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
$T_{\min} = 0.981$, $T_{\max} = 0.990$
4496 measured reflections
2442 independent reflections
1789 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.123$
$S = 1.14$
2442 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 1.15P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O14$^{\rm i}$	0.88	1.96	2.817 (2)	163

Symmetry code: (i) $-x+2, -y+1, -z$.

H atoms were located in a difference Fourier map and were subsequently included in the refinement in geometrically idealized positions, with C—H = 0.96–0.98 Å and N—H = 0.88 Å, and with $U_{\rm iso} = 1.2U_{\rm eq}$(C,N).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Blessing, R. H. (1997). *J. Appl. Cryst.* **30**, 421–426.
Fan, H.-F. (1991). *SAPI91*. Rigaku Corporation, Tokyo, Japan.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565
Frieden, M., Giraud, M., Reese, C. B. & Song, Q. (1998). *J. Chem. Soc. Perkin Trans. 1*, pp. 2827–2832.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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