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Key indicators

Single-crystal X-ray study
 $T = 292\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.044
 wR factor = 0.096
 Data-to-parameter ratio = 9.5

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

2-(4-Methoxyphenoxy)-1,9-diphenyl-1,9-dihydropurin-6-one

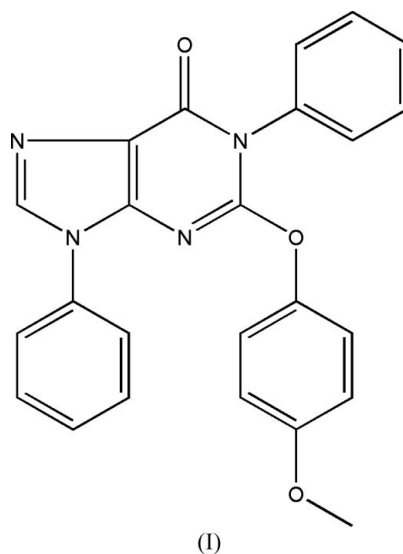
The title compound, $\text{C}_{24}\text{H}_{18}\text{N}_4\text{O}_3$, has a planar bicyclic imidazo[5,4-*d*]pyrimidine core. The planes of the phenyl and methoxyphenoxy substituents form substantial ($>30^\circ$) dihedral angles with the imidazolopyrimidine plane. Intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions link the molecules into infinite chains running along the *a* axis of the crystal structure.

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Comment

Due to the fundamental role of purines in nucleic acid chemistry and cellular biochemistry, the potential use of purine derivatives as chemotherapeutic agents in the treatment of malignant diseases was investigated as early as the 1930s (Lustig & Wachtel, 1935). Substituted guanine derivatives may be used as potential biologically active compounds or pharmaceuticals (Xu *et al.*, 1995). In recent years, we have been developing methods for the synthesis of derivatives of heterocycles *via* the aza-Wittig reaction (Ding *et al.*, 2004). In this context, we have synthesized the title compound, 2-(4-methoxyphenoxy)-1,9-diphenyl-1,9-dihydropurin-6-one, (I); here we report its crystal structure.



The molecular structure of (I) is shown in Fig. 1. Selected bond lengths and bond and torsion angles are listed in Table 1. The bicyclic imidazo[5,4-*d*]pyrimidine system is planar within 0.012 Å. The planes of the aromatic rings C2–C7, C9–C14 and C19–C24 form dihedral angles of 55.8 (1), 67.9 (1) and 34.2 (2)°, respectively, with the least-squares plane of the imidazolopyrimidine system; the N1–C8–O2–C5 and C8–O2–C5–C6 torsion angles are 18.8 (4) and 117.7 (3)°, respectively.

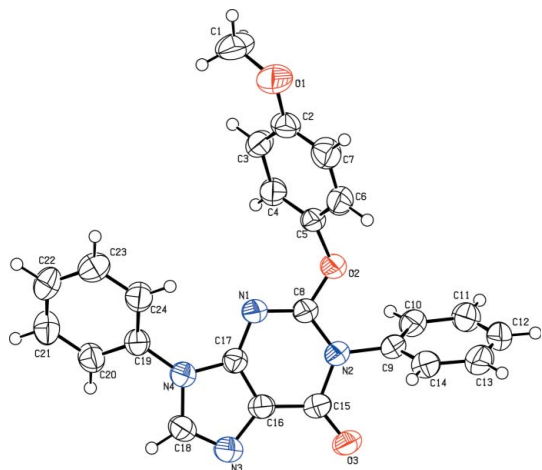


Figure 1
View of the molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

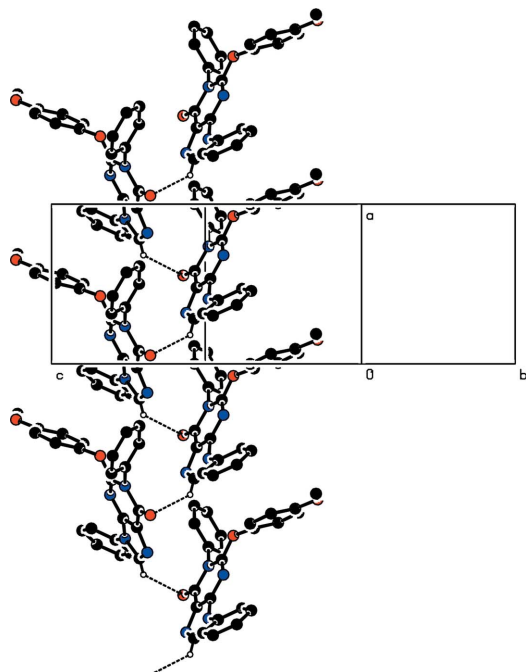


Figure 2
Packing diagram showing the crystal structure of the title compound. The C—H...O interactions are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Intermolecular C—H...O interactions (Table 2) link the molecules into infinite chains running along the *a* axis of the crystal structure (Fig. 2).

Experimental

Ethyl 5-[(phenylimino)methyleneamino]-1-phenylimidazole-4-carboxylate (2 mmol), 4-methoxyphenol (0.25 g) and potassium carbonate (0.1 g) were dissolved in dry acetonitrile (30 ml). The solution was stirred for 4 h at 310 K. The mixture was then filtered and the solvent was removed from the filtrate under reduced pressure. The solid residue was recrystallized from anhydrous ethanol

(10 ml) to produce the title compound, (I), in a yield of 83% (m.p. 470 K). Suitable crystals were obtained by vapor diffusion of dichloromethane into an ethanol solution at room temperature. MS (EI 70 eV) *m/z* (%): 410 (100), 379 (3), 303 (5), 291/287 (94/98), 275 (64), 231 (18), 76 (84). ¹H NMR (CDCl₃, 400 MHz): 7.98 (s, 1H, C—H), 7.51–7.55 (*m*, 5H, Ph—H), 7.37–7.41 (*m*, 5H, Ph—H), 6.83–7.05 (*m*, 4H, Ph—H), 3.79 (s, 1H, C—H).

Crystal data

C₂₄H₁₈N₄O₃
M_r = 410.42
Orthorhombic, *P*2₁2₁2₁
a = 8.0020 (7) Å
b = 9.7745 (8) Å
c = 25.255 (2) Å
V = 1975.3 (3) Å³
Z = 4
*D*_x = 1.380 Mg m⁻³

Mo Kα radiation
Cell parameters from 2809 reflections
 θ = 2.2–21.4°
 μ = 0.09 mm⁻¹
T = 292 (2) K
Block, colorless
0.30 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: none
12700 measured reflections
2677 independent reflections

1958 reflections with $I > 2\sigma(I)$
*R*_{int} = 0.061
 θ_{\max} = 28.0°
h = -10 → 10
k = -12 → 12
l = -23 → 32

Refinement

Refinement on *F*²
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.096$
S = 0.96
2677 reflections
281 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0474P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.14 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.20 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

C8—N1	1.300 (3)	C16—C17	1.366 (3)
C8—N2	1.374 (3)	C16—N3	1.386 (3)
C8—O2	1.340 (3)	C17—N1	1.362 (3)
C9—N2	1.451 (3)	C17—N4	1.375 (3)
C15—N2	1.427 (3)	C18—N3	1.306 (3)
C15—O3	1.220 (3)	C18—N4	1.379 (3)
C15—C16	1.428 (3)	C19—N4	1.434 (3)
N1—C8—O2	122.4 (2)	C16—C17—N4	106.0 (2)
O2—C8—N2	111.1 (2)	N3—C18—N4	114.1 (2)
O3—C15—N2	120.5 (2)	C8—N1—C17	111.75 (19)
O3—C15—C16	128.5 (2)	C8—N2—C15	122.7 (2)
N2—C15—C16	110.99 (19)	C8—N2—C9	120.0 (2)
C17—C16—N3	111.5 (2)	C15—N2—C9	117.23 (18)
C17—C16—C15	120.0 (2)	C18—N3—C16	103.2 (2)
N3—C16—C15	128.4 (2)	C17—N4—C18	105.07 (19)
N1—C17—C16	128.0 (2)	C17—N4—C19	130.3 (2)
N1—C17—N4	126.0 (2)	C18—N4—C19	124.6 (2)
O3—C15—C16—C17	-179.5 (2)	C14—C9—N2—C8	111.6 (3)
O3—C15—C16—N3	1.4 (4)	C10—C9—N2—C15	110.8 (3)
N2—C15—C16—N3	-178.9 (2)	C14—C9—N2—C15	-68.5 (3)
N3—C16—C17—N1	179.3 (2)	C20—C19—N4—C17	143.9 (3)
C15—C16—C17—N1	0.0 (4)	C24—C19—N4—C17	-37.7 (4)
N3—C16—C17—N4	-0.5 (3)	C20—C19—N4—C18	-32.8 (4)
C15—C16—C17—N4	-179.8 (2)	C24—C19—N4—C18	145.6 (3)
O2—C8—N1—C17	-179.3 (2)	N1—C8—O2—C5	18.8 (4)
N4—C17—N1—C8	179.4 (2)	N2—C8—O2—C5	-161.1 (2)
O2—C8—N2—C15	179.5 (2)	C6—C5—O2—C8	117.7 (3)
C10—C9—N2—C8	-69.1 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C18—H18 \cdots O3 ⁱ	0.93	2.58	3.315 (3)	137

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 2$.

The H atoms were placed in calculated positions and treated as riding atoms ($C-H = 0.93-0.98 \text{ \AA}$) with $U_{iso}(H)$ values set at $1.2U_{eq}(C)$ for aromatic and $1.5U_{eq}(C)$ for methyl H atoms. In the absence of significant anomalous scattering, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

SHELXTL (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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