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2-(Biphenyl-4-yl)-2,3-dihydroquinazolin-4(1*H*)-one

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Key indicators

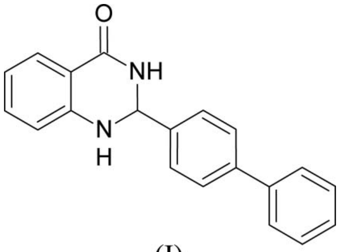
Single-crystal X-ray study
T = 103 K
Mean σ(C–C) = 0.002 Å
R factor = 0.055
wR factor = 0.165
Data-to-parameter ratio = 15.6

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

All N and O atoms in the title structure, $C_{20}H_{16}N_2O$, are involved in hydrogen bonding. The benzene rings in the biphenyl fragment are rotated with respect to each other, the angle between their planes being 11.3 (1)°.

Comment

The title compound, (I), is a member of the quinazolinone family which has been shown to have varied biological and pharmacological activities. The quinazolinone unit is present in alkaloids and their precursors (Möhrle & Gundlach, 1970; Liu *et al.*, 2006) and is also considered to be a privileged structure in drug discovery (Horton *et al.*, 2003). There are many examples showing the varied pharmacological activities of quinazolinone derivatives. For example, they exhibit diuretic (Cohen *et al.*, 1960), anti-inflammatory (Saravanan *et al.*, 1998), choleretic (Bonola *et al.*, 1968) and anticancer activities (Hour *et al.*, 2000; Carrico *et al.*, 2005). Compound (I) was synthesized as an analog in an anticancer drug discovery program.



(I)

The molecular structure of (I) is shown in Fig. 1. There is a chiral center at carbon C2 and the crystal is a racemate. Although quinazolinone derivatives are quite well represented in the November 2006 release of the Cambridge Structural Database (Allen, 2002), there are only few structures in which both NH groups of the 4(1*H*,3*H*)-quinazolinone fragment are unsubstituted.

In the crystal structure of (I), the benzene rings in the biphenyl fragment are slightly twisted with respect to each other (Table 1); the torsion angle C13—C14—C17—C18 has a value of −10.2 (3)°, while the angle between the planes of the rings is 11.3 (1)°.

All N and O atoms are involved in hydrogen bonds (Fig. 2), and atom O1 is an acceptor for two hydrogen bonds. The geometric parameters describing the hydrogen bonds are summarized in Table 2. Hydrogen bonds, together with weak van der Waals interactions, play the most important role in the stabilization of the crystal structure. The NHCO group acts as both the donor and the acceptor of the hydrogen bonds that form centrosymmetric dimers of (I).

Experimental

The title compound was synthesized as described previously (Brown, 2002). The crystal used for the X-ray experiment was grown from a solution of a 1:1 mixture of 1-butanol and 2-propanol by slow evaporation. Crystallization was performed at 293 K.

Crystal data

$C_{20}H_{16}N_2O$
$M_r = 300.35$
Monoclinic, $P2_1/c$
$a = 15.485$ (1) Å
$b = 9.025$ (1) Å
$c = 11.042$ (1) Å
$\beta = 96.18$ (1)°
$V = 1534.2$ (2) Å^3
$Z = 4$
$D_x = 1.300$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 103$ (2) K
Plate, colorless
0.50 × 0.45 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans with χ offset
Absorption correction: multi-scan (Otwinowski *et al.*, 2003)
$T_{\min} = 0.95$, $T_{\max} = 0.99$
29267 measured reflections
3373 independent reflections
2971 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.055$
$\theta_{\max} = 27.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.165$
$S = 1.04$
3373 reflections
216 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0934P)^2 + 0.711P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.55$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

Table 1
Selected torsion angles (°).

C2—N3—C4—C10	−13.0 (2)	C12—C11—C2—N1	−126.7 (2)
C2—N1—C9—C10	33.8 (2)	C16—C11—C2—N1	55.9 (2)
C9—N1—C2—N3	−50.0 (2)	C12—C11—C2—N3	114.1 (2)
C9—N1—C2—C11	−169.7 (1)	C16—C11—C2—N3	−63.3 (2)
C4—N3—C2—N1	41.1 (2)	C18—C17—C14—C13	−10.2 (3)
C4—N3—C2—C11	162.8 (1)	C18—C17—C14—C15	169.3 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1$^{\rm i}$	0.88 (2)	2.00 (2)	2.878 (2)	176 (2)
N1—H1···O1$^{\rm ii}$	0.87 (2)	2.21 (2)	2.997 (2)	151 (2)

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

H atoms attached to N atoms were located in a difference map and all their parameters were refined. All H atoms bound to C atoms were placed in geometric positions and treated as riding, with aromatic C—H = 0.93 Å, C2—H = 0.98 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

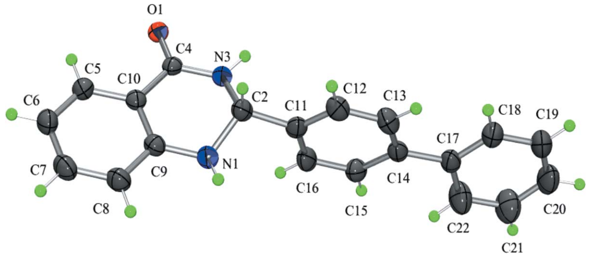


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as green spheres of an arbitrary radius.

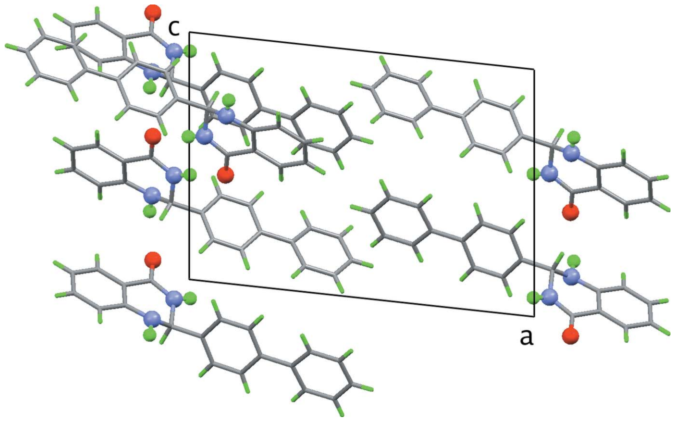


Figure 2
The crystal packing of compound (I), shown along [010]. The atoms forming the hydrogen-bond network are marked as spheres and H atoms are shown in green.

Data collection: *HKL-2000* (Otwinowski & Minor, 1997); cell refinement: *HKL-2000*; data reduction: *HKL-2000*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997) and *HKL-3000SM* (Minor *et al.*, 2006); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997) and *HKL*-3000SM; molecular graphics: *HKL*-3000SM, *Mercury* (Macrae *et al.*, 2006) *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3* (Farrugia, 1997) and *POV-RAY* (The *POV-RAY* Team, 2004); software used to prepare material for publication: *HKL-3000SM*.

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