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2-(1*H*-Benzimidazol-1-yl)-1-(2-furyl)-3-phenylpropan-1-one

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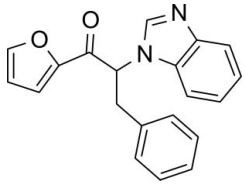
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.127; data-to-parameter ratio = 11.9.

In the molecule of the title compound, $C_{20}H_{16}N_2O_2$, the planar benzimidazole system is oriented with respect to the furan and phenyl rings with dihedral angles of 87.41 (10) and 61.65 (5)°, respectively. In the crystal structure, intermolecular C—H···O and C—H···N hydrogen bonds link the molecules to form a network structure.

Related literature

For general background, see: Mann *et al.* (2001); Chen *et al.* (1993); Evans *et al.* (1996); Roth *et al.* (1997); Saito *et al.* (1993); Awouters *et al.* (1983); Brandstrom *et al.* (1985); Preston (1974); Cozzi *et al.* (1994). For related literature, see: Özel Güven *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{16}N_2O_2$
M_r = 316.35
Monoclinic, $P2_1/n$
a = 16.3886 (2) Å
b = 6.5976 (2) Å
c = 16.7166 (3) Å
β = 114.677 (9)°
V = 1642.42 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.35 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.971, T_{max} = 0.983
3451 measured reflections
3334 independent reflections
1884 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.127
S = 0.99
3334 reflections
281 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O2	0.97 (2)	2.35 (2)	3.250 (3)	154.9 (17)
C19—H19···N2^{i}	0.92 (3)	2.61 (3)	3.529 (3)	170.4 (18)

Symmetry codes: (i) $x, y+1, z$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2303).

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supplementary materials

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2-(1*H*-Benzimidazol-1-yl)-1-(2-furyl)-3-phenylpropan-1-one

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Comment

In recent years, the benzimidazole heterocyclic ring system has attracted considerable attention, due to its useful properties for the development of interesting new pharmaceutical compounds (Mann *et al.*, 2001). Some of the substituted benzimidazole derivatives have antitumour, antiviral, antibacterial, anti-inflammatory (Roth *et al.*, 1997; Evans *et al.*, 1996; Chen *et al.*, 1993) and therapeutic (Saito *et al.*, 1993; Awouters *et al.*, 1983; Brandstrom *et al.*, 1985) activities. On the other hand, a series of benzimidazole derivatives are useful for central nervous system disorders (Preston, 1974). In literature, 2-(1*H*-imidazol-1-yl)-1,3-diphenylpropan-1-one and its derivatives have been reported that they show both high and selective thromboxane A2 receptor antagonist and thromboxane A2 synthase inhibitory activities (Cozzi *et al.*, 1994). The structure determination of the title molecule, (I) was carried out in order to investigate the strength of the hydrogen bonding capability of the benzimidazole heterocyclic ring system.

In the molecule of the title compound (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). A (O1/C1—C4), B (C8—C13), C(N1/N2/C14/C15/C20) and D (C15—C20) rings are, of course, planar and the dihedral angles between the rings are A/B = 47.64 (11)° and C/D = 1.52 (8)°. Thus, the benzimidazole ring system E (N1/N2/C14—C20) is also planar and it is oriented with respect to rings A and B at dihedral angles of A/E = 87.41 (10)° and B/E = 61.65 (5)°.

In the crystal structure, intermolecular C—H···O and C—H···N hydrogen bonds (Table 1) link the molecules to form a network structure (Fig. 2), in which they seem to be effective in the stabilization of the structure.

Experimental

The title compound was synthesized as a byproduct in one-pot reaction from 2-(1*H*-benzimidazol-1-yl)-1-(furan-2-yl)ethanone (Özel Güven *et al.*, 2007) (0.1 g, 0.44 mmol), hydroxylamine hydrogenchloride (0.037 g, 0.53 mmol), benzyl bromide (0.091 g, 0.53 mmol) and KOH (0.213 g, 3.8 mmol) in DMSO (0.53 ml) and water (0.22 ml). Reaction was completed in half an hour at room temperature by stirring. Then, ethyl acetate (3 ml) and brine (1 ml) were added and the reaction mixture was extracted with ethyl acetate. The organic layer was washed with brine three times, dried, filtered and evaporated. The crude residue was purified by column chromatography and recrystallized from methanol to obtain pink crystals (yield; 28 mg, 20%).

Refinement

H atoms were located in difference syntheses and refined isotropically [C—H = 0.88 (2)–0.93 (3) Å, U_{iso}(H) = 0.027 (4)–0.111 (10) Å^2].

Figures

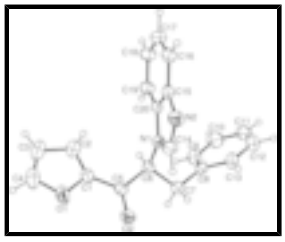

Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

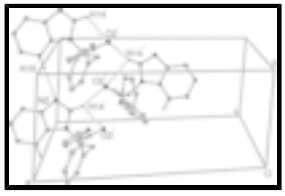

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity [symmetry codes: (') $-x, -y, -z$; (") $x + 1/2, -y + 1/2, z + 1/2$].

2-(1*H*-Benzimidazol-1-yl)-1-(2-furyl)-3-phenylpropan-1-one

Crystal data

$C_{20}H_{16}N_2O_2$	F_{000} = 664
M_r = 316.35	D_x = 1.279 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 426-427 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 16.3886 (2) Å	Cell parameters from 25 reflections
b = 6.5976 (2) Å	θ = 2.3–19.5º
c = 16.7166 (3) Å	μ = 0.08 mm^{-1}
β = 114.677 (9)º	T = 298 (2) K
V = 1642.42 (13) Å^3	Prism, pink
Z = 4	0.35 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer	R_{int} = 0.020
Radiation source: fine-focus sealed tube	θ_{max} = 26.3º
Monochromator: graphite	θ_{min} = 2.9º
T = 298(2) K	h = −20→0
Non–profiled ω scans	k = 0→8
Absorption correction: ψ scan (North *et al.*, 1968)	l = −18→20
T_{min} = 0.971, T_{max} = 0.983	3 standard reflections
3451 measured reflections	every 120 min
3334 independent reflections	intensity decay: 1%
1884 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	All H-atom parameters refined
$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.2297P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
3334 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
281 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.16659 (12)	1.0691 (3)	0.07170 (10)	0.0713 (5)
O2	1.25039 (11)	0.9637 (2)	0.24119 (10)	0.0587 (4)
N1	1.06934 (11)	0.9260 (2)	0.26597 (10)	0.0416 (4)
N2	1.01229 (13)	0.6120 (3)	0.24342 (13)	0.0586 (5)
C1	1.13037 (15)	1.1210 (3)	0.12921 (13)	0.0491 (5)
C2	1.05646 (19)	1.2327 (4)	0.08763 (16)	0.0654 (7)
H2	1.0208 (15)	1.281 (3)	0.1103 (15)	0.059 (7)*
C3	1.0455 (3)	1.2498 (5)	−0.00107 (17)	0.0817 (9)
H3	0.997 (2)	1.315 (5)	−0.040 (2)	0.108 (11)*
C4	1.1125 (3)	1.1502 (5)	−0.00629 (18)	0.0827 (9)
H4	1.1326 (18)	1.122 (4)	−0.0526 (18)	0.092 (9)*
C5	1.17906 (14)	1.0521 (3)	0.21829 (13)	0.0435 (5)
C6	1.13654 (13)	1.0859 (3)	0.28278 (12)	0.0408 (5)
H6	1.1044 (11)	1.215 (3)	0.2708 (10)	0.027 (4)*
C7	1.20677 (15)	1.0837 (4)	0.37823 (13)	0.0503 (6)
H71	1.2514 (13)	1.187 (3)	0.3809 (13)	0.057 (6)*
H72	1.2361 (13)	0.952 (3)	0.3899 (13)	0.054 (6)*
C8	1.16775 (13)	1.1282 (3)	0.44258 (12)	0.0475 (5)

C9	1.14102 (18)	1.3217 (4)	0.45064 (17)	0.0668 (7)
H9	1.1472 (17)	1.423 (4)	0.4145 (18)	0.088 (9)*
C10	1.1036 (2)	1.3656 (6)	0.50851 (19)	0.0822 (9)
H10	1.0870 (18)	1.502 (4)	0.5123 (17)	0.085 (9)*
C11	1.09365 (19)	1.2166 (7)	0.56044 (18)	0.0858 (10)
H11	1.0705 (19)	1.237 (5)	0.602 (2)	0.111 (10)*
C12	1.1206 (2)	1.0237 (7)	0.55359 (19)	0.0863 (9)
H12	1.114 (2)	0.919 (4)	0.588 (2)	0.106 (10)*
C13	1.15763 (18)	0.9805 (5)	0.49538 (16)	0.0674 (7)
H13	1.1757 (17)	0.847 (4)	0.4899 (16)	0.084 (9)*
C14	1.08385 (16)	0.7231 (3)	0.26522 (15)	0.0530 (6)
H14	1.1436 (14)	0.672 (3)	0.2790 (13)	0.057 (6)*
C15	0.94413 (13)	0.7514 (3)	0.22835 (12)	0.0453 (5)
C16	0.85217 (15)	0.7207 (4)	0.20142 (15)	0.0567 (6)
H16	0.8277 (15)	0.585 (4)	0.1919 (14)	0.062 (7)*
C17	0.79920 (17)	0.8872 (4)	0.18858 (16)	0.0636 (7)
H17	0.7355 (17)	0.866 (4)	0.1711 (15)	0.079 (7)*
C18	0.83400 (16)	1.0828 (4)	0.20143 (17)	0.0631 (7)
H18	0.7947 (17)	1.201 (4)	0.1940 (17)	0.088 (8)*
C19	0.92461 (15)	1.1180 (4)	0.22888 (15)	0.0521 (6)
H19	0.9489 (14)	1.247 (4)	0.2400 (14)	0.066 (7)*
C20	0.97822 (13)	0.9480 (3)	0.24149 (11)	0.0393 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0881 (12)	0.0851 (12)	0.0518 (10)	−0.0060 (10)	0.0402 (9)	−0.0032 (9)
O2	0.0528 (9)	0.0628 (10)	0.0674 (10)	0.0076 (8)	0.0318 (8)	0.0094 (8)
N1	0.0399 (9)	0.0418 (10)	0.0434 (9)	−0.0024 (8)	0.0176 (7)	0.0033 (8)
N2	0.0565 (12)	0.0452 (11)	0.0743 (13)	−0.0032 (10)	0.0275 (10)	0.0071 (10)
C1	0.0563 (13)	0.0509 (13)	0.0440 (12)	−0.0088 (12)	0.0249 (11)	−0.0027 (10)
C2	0.0739 (17)	0.0653 (17)	0.0517 (14)	0.0044 (15)	0.0210 (13)	0.0042 (13)
C3	0.101 (2)	0.078 (2)	0.0484 (16)	−0.0015 (19)	0.0126 (16)	0.0119 (15)
C4	0.117 (3)	0.085 (2)	0.0481 (16)	−0.014 (2)	0.0369 (17)	−0.0003 (15)
C5	0.0432 (12)	0.0399 (11)	0.0480 (12)	−0.0070 (10)	0.0195 (10)	0.0007 (10)
C6	0.0400 (11)	0.0416 (12)	0.0410 (11)	−0.0025 (10)	0.0170 (9)	0.0029 (9)
C7	0.0432 (12)	0.0614 (16)	0.0436 (12)	−0.0022 (13)	0.0155 (10)	0.0028 (11)
C8	0.0415 (11)	0.0593 (14)	0.0349 (11)	−0.0042 (11)	0.0093 (9)	0.0007 (10)
C9	0.0748 (18)	0.0720 (19)	0.0566 (15)	−0.0004 (15)	0.0304 (14)	0.0013 (14)
C10	0.081 (2)	0.094 (2)	0.0724 (19)	0.0038 (18)	0.0335 (16)	−0.0170 (18)
C11	0.0634 (17)	0.150 (3)	0.0486 (15)	−0.006 (2)	0.0277 (14)	−0.011 (2)
C12	0.083 (2)	0.122 (3)	0.0592 (17)	−0.004 (2)	0.0354 (16)	0.0227 (19)
C13	0.0724 (17)	0.076 (2)	0.0540 (14)	0.0010 (15)	0.0261 (13)	0.0160 (13)
C14	0.0489 (14)	0.0441 (14)	0.0669 (15)	0.0061 (12)	0.0249 (12)	0.0102 (11)
C15	0.0466 (12)	0.0498 (13)	0.0399 (11)	−0.0031 (11)	0.0184 (9)	0.0049 (10)
C16	0.0494 (14)	0.0606 (16)	0.0579 (14)	−0.0130 (13)	0.0200 (11)	0.0029 (12)
C17	0.0427 (14)	0.082 (2)	0.0648 (15)	−0.0060 (14)	0.0208 (12)	0.0016 (14)
C18	0.0493 (15)	0.0658 (18)	0.0775 (17)	0.0058 (13)	0.0296 (13)	−0.0001 (14)

C19	0.0491 (13)	0.0490 (15)	0.0611 (14)	0.0015 (12)	0.0259 (11)	−0.0028 (12)
C20	0.0382 (11)	0.0483 (12)	0.0334 (10)	−0.0022 (10)	0.0171 (8)	0.0020 (9)

Geometric parameters (Å, °)

O1—C1	1.368 (2)	C9—C10	1.375 (4)
O1—C4	1.344 (3)	C9—H9	0.93 (3)
O2—C5	1.216 (2)	C10—H10	0.95 (3)
N1—C6	1.465 (2)	C11—C10	1.366 (4)
N1—C14	1.361 (3)	C11—C12	1.367 (5)
N2—C14	1.299 (3)	C11—H11	0.93 (3)
N2—C15	1.386 (3)	C12—H12	0.94 (3)
C1—C2	1.338 (3)	C13—C12	1.375 (4)
C2—C3	1.422 (4)	C13—H13	0.94 (3)
C2—H2	0.88 (2)	C14—H14	0.97 (2)
C3—H3	0.90 (3)	C15—C16	1.396 (3)
C4—C3	1.314 (4)	C16—H16	0.97 (2)
C4—H4	0.98 (3)	C17—C16	1.361 (3)
C5—C1	1.438 (3)	C17—C18	1.390 (4)
C6—C5	1.525 (3)	C17—H17	0.97 (2)
C6—C7	1.529 (3)	C18—C19	1.379 (3)
C6—H6	0.979 (17)	C18—H18	0.99 (3)
C7—C8	1.492 (3)	C19—H19	0.93 (2)
C7—H71	0.99 (2)	C20—N1	1.382 (2)
C7—H72	0.97 (2)	C20—C15	1.393 (3)
C8—C9	1.375 (3)	C20—C19	1.385 (3)
C8—C13	1.370 (3)		
C4—O1—C1	106.1 (2)	C8—C9—H9	118.3 (17)
C14—N1—C20	105.79 (17)	C10—C9—H9	120.4 (17)
C14—N1—C6	126.14 (18)	C11—C10—C9	120.1 (3)
C20—N1—C6	127.91 (17)	C11—C10—H10	121.7 (17)
C14—N2—C15	103.98 (18)	C9—C10—H10	118.1 (17)
C2—C1—O1	109.7 (2)	C10—C11—C12	119.2 (3)
C2—C1—C5	134.6 (2)	C10—C11—H11	124 (2)
O1—C1—C5	115.6 (2)	C12—C11—H11	116 (2)
C1—C2—C3	106.2 (3)	C11—C12—C13	120.4 (3)
C1—C2—H2	126.6 (15)	C11—C12—H12	120.7 (19)
C3—C2—H2	127.2 (15)	C13—C12—H12	118.9 (19)
C4—C3—C2	106.5 (3)	C8—C13—C12	121.1 (3)
C4—C3—H3	135 (2)	C8—C13—H13	118.2 (16)
C2—C3—H3	119 (2)	C12—C13—H13	120.7 (16)
C3—C4—O1	111.5 (3)	N2—C14—N1	114.6 (2)
C3—C4—H4	135.7 (16)	N2—C14—H14	125.1 (13)
O1—C4—H4	112.8 (16)	N1—C14—H14	120.2 (13)
O2—C5—C1	121.48 (19)	N2—C15—C20	110.44 (17)
O2—C5—C6	120.70 (18)	N2—C15—C16	129.9 (2)
C1—C5—C6	117.77 (19)	C20—C15—C16	119.6 (2)
N1—C6—C5	106.74 (15)	C17—C16—C15	117.7 (2)
N1—C6—C7	111.81 (16)	C17—C16—H16	121.9 (13)

C5—C6—C7	111.68 (17)	C15—C16—H16	120.3 (13)
N1—C6—H6	106.9 (9)	C16—C17—C18	122.1 (2)
C5—C6—H6	110.4 (9)	C16—C17—H17	117.9 (15)
C7—C6—H6	109.2 (9)	C18—C17—H17	120.0 (15)
C8—C7—C6	112.83 (18)	C19—C18—C17	121.5 (2)
C8—C7—H71	111.3 (12)	C19—C18—H18	117.7 (15)
C6—C7—H71	105.1 (12)	C17—C18—H18	120.7 (15)
C8—C7—H72	110.9 (12)	C18—C19—C20	116.2 (2)
C6—C7—H72	108.1 (12)	C18—C19—H19	122.3 (14)
H71—C7—H72	108.2 (16)	C20—C19—H19	121.6 (14)
C13—C8—C9	117.9 (2)	N1—C20—C19	131.96 (19)
C13—C8—C7	121.9 (2)	N1—C20—C15	105.17 (17)
C9—C8—C7	120.2 (2)	C19—C20—C15	122.86 (19)
C8—C9—C10	121.2 (3)		
C4—O1—C1—C2	−0.6 (3)	C6—C7—C8—C13	107.3 (3)
C4—O1—C1—C5	−178.9 (2)	C6—C7—C8—C9	−73.0 (3)
C1—O1—C4—C3	0.3 (3)	C13—C8—C9—C10	−1.3 (4)
C14—N1—C6—C5	54.1 (2)	C7—C8—C9—C10	179.0 (2)
C20—N1—C6—C5	−120.7 (2)	C9—C8—C13—C12	1.0 (4)
C14—N1—C6—C7	−68.3 (3)	C7—C8—C13—C12	−179.3 (2)
C20—N1—C6—C7	116.9 (2)	C8—C9—C10—C11	1.1 (4)
C6—N1—C14—N2	−176.05 (17)	C12—C11—C10—C9	−0.5 (4)
C20—N1—C14—N2	−0.3 (3)	C10—C11—C12—C13	0.3 (5)
C15—N2—C14—N1	−0.1 (3)	C8—C13—C12—C11	−0.5 (4)
C14—N2—C15—C20	0.4 (2)	N2—C15—C16—C17	−177.7 (2)
C14—N2—C15—C16	178.7 (2)	C20—C15—C16—C17	0.4 (3)
O1—C1—C2—C3	0.6 (3)	C18—C17—C16—C15	0.0 (4)
C5—C1—C2—C3	178.5 (2)	C16—C17—C18—C19	−0.7 (4)
C1—C2—C3—C4	−0.3 (3)	C17—C18—C19—C20	0.9 (4)
O1—C4—C3—C2	0.0 (3)	C19—C20—N1—C14	−178.3 (2)
O2—C5—C1—C2	−173.7 (2)	C15—C20—N1—C14	0.6 (2)
C6—C5—C1—C2	8.6 (4)	C19—C20—N1—C6	−2.7 (3)
O2—C5—C1—O1	4.1 (3)	C15—C20—N1—C6	176.18 (17)
C6—C5—C1—O1	−173.56 (17)	N1—C20—C15—N2	−0.6 (2)
N1—C6—C5—O2	−98.0 (2)	C19—C20—C15—N2	178.35 (19)
C7—C6—C5—O2	24.5 (3)	N1—C20—C15—C16	−179.07 (17)
N1—C6—C5—C1	79.6 (2)	C19—C20—C15—C16	−0.1 (3)
C7—C6—C5—C1	−157.90 (19)	N1—C20—C19—C18	178.1 (2)
N1—C6—C7—C8	−63.7 (3)	C15—C20—C19—C18	−0.5 (3)
C5—C6—C7—C8	176.73 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O2^{i}	0.97 (2)	2.35 (2)	3.250 (3)	154.9 (17)
C19—H19···N2^{ii}	0.92 (3)	2.61 (3)	3.529 (3)	170.4 (18)

Symmetry codes: (i) , −1, ; (ii) *x*, *y*+1, *z*.

Fig. 1

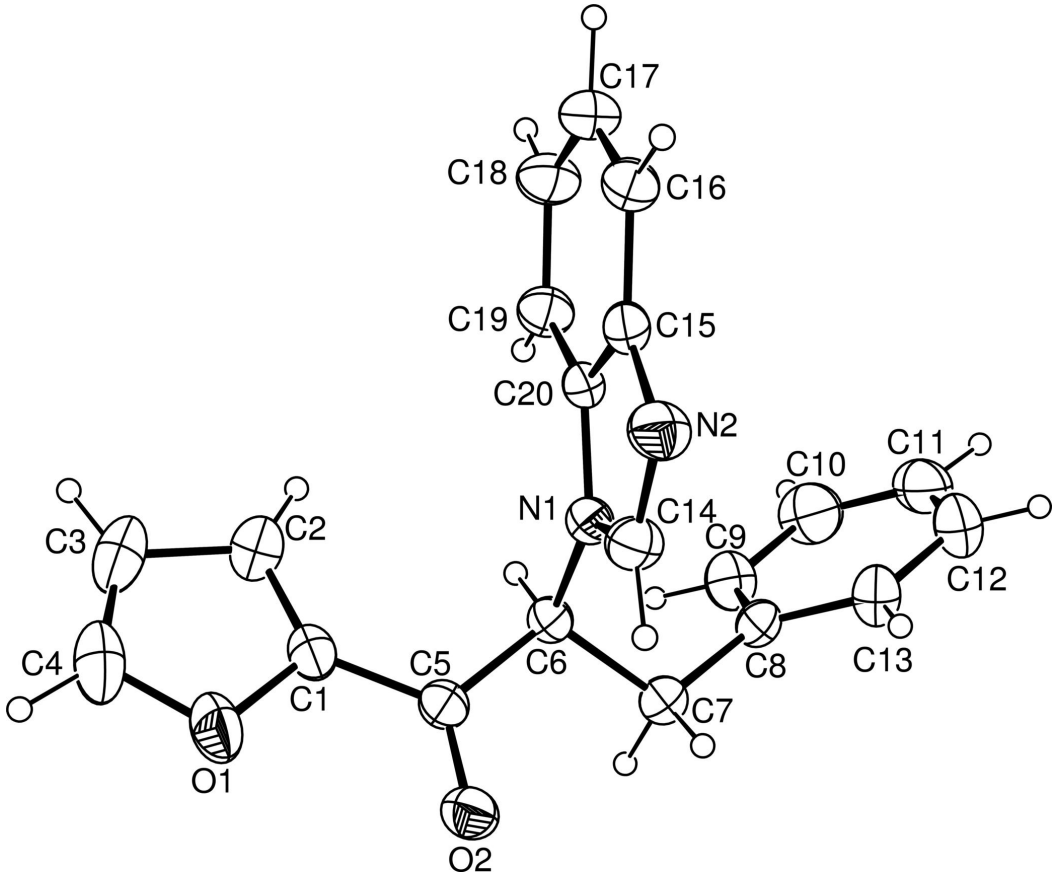
C17
C18
C16
C19
C15
C20
N2
C11
C10
N1
C14
C2
C3
C9
C12
C4
C5
C6
C8
C13
C1
C7
O1
O2

Fig. 2