Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(±)-2-Benzoyl-8-ethyl-1,2-dihydroisoquinoline-1-carbonitrile: an original Reissert compound

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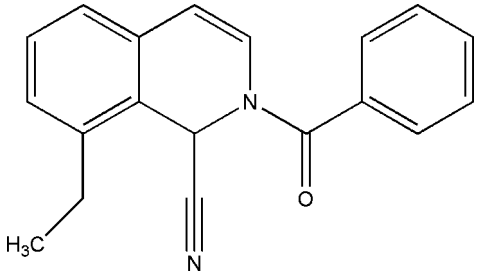
Received 1 June 2007; accepted 6 June 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.133; data-to-parameter ratio = 15.3.

The title compound, $C_{19}H_{16}N_2O$, is a Reissert compound. The heterocyclic fragment of the molecule exhibits a 1,3-diplanar conformation. The phenyl ring is connected to the isoquinoline ring system *via* an amide bond that adopts an *anti* conformation with respect to the adjacent C—N bond in the adjacent heterocyclic ring. Intra- and intermolecular C—H···O hydrogen bonds are present in the crystal structure.

Related literature

For related literature, see: Cooney (1983); Hendrickson & Rodriguez (1983); Pływaczyk *et al.* (1984); Ruchirawat *et al.* (1977); Tykarska *et al.* (1985).



Experimental

Crystal data

$C_{19}H_{16}N_2O$
M_r = 288.34
Triclinic, $P\overline{1}$
a = 7.996 (1) Å
b = 8.948 (1) Å
c = 11.297 (2) Å
α = 108.51 (2)°
β = 94.86 (1)°
γ = 93.04 (1)°
V = 761.0 (2) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.62 mm^{-1}
T = 293 K
0.25 × 0.19 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.870, T_{max} = 0.912
3363 measured reflections
3129 independent reflections
2863 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.07
3129 reflections
204 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1	0.952 (16)	2.297 (16)	2.6471 (17)	100.9 (11)
C8—H8···O1^{i}	0.93	2.57	3.4083 (17)	151

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

Data collection: locally modified *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *SET4* (de Boer & Duisenberg, 1984); data reduction: *HELENA* (Spek, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

AG was supported by a PhD fellowship of the FRIA (Belgium). JFL is a Senior Research Associate of the FNRS (Belgium). Financial support by FRSM grant No. 3.4566.03 and from the Léon Frédéricq Foundation is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2150).

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 doi:10.1107/S1600536807027729

supplementary materials

Acta Cryst. (2007). E**63**, o3161 [**doi:10.1107/S1600536807027729**]

(±)-2-Benzoyl-8-ethyl-1,2-dihydroisoquinoline-1-carbonitrile: an original Reissert compound

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Comment

Reissert compounds are of major synthetic interest as reagents for different synthetic pathways, such as alkylation, condensation with aldehydes and ketones, rearrangements and conjugate additions (Cooney, 1983).

2-Benzoyl-1-cyano-8-ethyl-1,2-dihydroisoquinoline, is a Reissert compound. As expected, bond lengths and angles are similar to those observed in the analogue with no ethyl group at C4 (Tykarska *et al.*, 1985). All bond lengths of the nitrogen-containing six-membered ring of the isoquinoline group are different, ranging from 1.330 (2) Å to 1.515 (2)Å and are significantly different from those observed in the tetrahydrogenated non-ethylated derivative (Pływaczyk *et al.*, 1984). Bond angles at N1, C5, C7, C8, C9 (ranging from 116.3 (1)° to 121.1 (1)°) are typical for sp^2 hybridization. The N1—C6—C5 angle is significantly smaller (111.7 (1)°), approaching, as expected, the classical value for an sp^3 hybridization. The heterocyclic ring molecule exhibits a 1,3-diplanar conformation.

The phenyl ring is connected to the isoquinoline unit *via* an amide bond that adopts an anti conformation with respect to the adjacent C7—N1 bond. Coplanarity of the aromatic system of the isoquinoline moiety and the amide group allows maximum conjugation. In contrast, the amide group and the phenyl ring are not conjugated, with an N1—C10—C11—C12 torsion angle of 140.6 (1)°. A similar conformation is observed for the unsubstituted analogue, 2-benzoyl-1-cyano-1,2-dihydroisoquinoline.

Interestingly, the ethyl group is almost perpendicular to the dihydroisoquinoline system (C3—C4—C17—C18 = −105.7 (2)°) and points in the same direction as the cyano group.

Experimental

The title compound, (±)-2-benzoyl-1-cyano-8-ethyl-1,2-dihydroisoquinoline, was obtained by reaction of 8-ethylisoquinoline with benzoyl chloride and trimethylsilyl cyanide in anhydrous dichloromethane (Ruchirawat *et al.*, 1977).

8-Ethylisoquinoline was prepared from 2-ethylbenzaldehyde by the Hendrickson modification of the Pomeranz-Fritsch synthesis (Hendrickson & Rodriguez, 1983).

Crystals were obtained by slow evaporation of a methanol solution at room temperature.

Refinement

H6, attached to C6, was located in a difference map and refined freely. All other H atoms were placed at idealized positions and allowed to ride on their parent atoms, with C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene groups, C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic carbons, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl group.

Figures

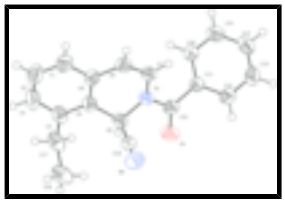


Fig. 1. The molecular structure of the title compound, with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

(±)-2-Benzoyl-8-ethyl-1,2-dihydroisoquinoline-1-carbonitrile

Crystal data

$C_{19}H_{16}N_2O$	V = 761.0 (2) Å^3
M_r = 288.34	Z = 2
Triclinic, $P\bar{1}$	F_{000} = 304
Hall symbol: -P 1	Least Squares Treatment of 25 SET4 setting angles.
a = 7.996 (1) Å	D_x = 1.258 Mg m^{-3}
b = 8.948 (1) Å	Cu $K\alpha$ radiation λ = 1.54178 Å
c = 11.297 (2) Å	μ = 0.62 mm^{-1}
α = 108.51 (2)º	T = 293 K
β = 94.86 (1)º	Prism, colourless
γ = 93.04 (1)º	0.25 × 0.19 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.016
Radiation source: sealed tube	θ_{max} = 75.1º
Monochromator: graphite	θ_{min} = 4.2º
T = 293 K	h = 0→10
profile data from θ/2θ scans	k = −11→11
Absorption correction: analytical (de Meulenaer & Tompa, 1965)	l = −14→14
T_{min} = 0.870, T_{max} = 0.912	3 standard reflections
3363 measured reflections	every 60 min
3129 independent reflections	intensity decay: 0.03%
2863 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
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.133	$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.146P]$

	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.002
3129 reflections	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
204 parameters	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit S are based on F2, conventional *R*-factors *R* are based on F, with F set to zero for negative F2. The observed criterion of F2 > 2sigma(F2) is used only for calculating –*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F2 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	0.90833 (12)	0.53709 (13)	0.34650 (11)	0.0621 (3)
N1	0.62678 (12)	0.54197 (12)	0.32412 (9)	0.0387 (3)
N2	0.6167 (2)	0.15692 (17)	0.30988 (14)	0.0725 (5)
C1	0.16240 (19)	0.39167 (19)	0.10521 (15)	0.0571 (5)
C2	0.1597 (2)	0.3137 (2)	−0.02105 (17)	0.0689 (6)
C3	0.3059 (2)	0.2683 (2)	−0.07305 (14)	0.0633 (5)
C4	0.46169 (19)	0.29521 (15)	0.00046 (12)	0.0480 (4)
C5	0.46170 (16)	0.37120 (14)	0.12923 (11)	0.0390 (3)
C6	0.61905 (16)	0.39340 (14)	0.21979 (11)	0.0399 (3)
C7	0.47592 (15)	0.57954 (14)	0.37858 (12)	0.0394 (3)
C8	0.32744 (16)	0.51787 (15)	0.31459 (12)	0.0426 (4)
C9	0.31451 (16)	0.42280 (15)	0.18231 (12)	0.0421 (4)
C10	0.78571 (15)	0.60681 (15)	0.38120 (12)	0.0416 (4)
C11	0.80173 (15)	0.76349 (14)	0.48144 (11)	0.0390 (3)
C12	0.91843 (17)	0.78653 (17)	0.58549 (14)	0.0515 (4)
C13	0.9493 (2)	0.9350 (2)	0.67430 (15)	0.0610 (5)
C14	0.8673 (2)	1.06002 (18)	0.65893 (15)	0.0576 (5)
C15	0.7526 (2)	1.03744 (17)	0.55620 (14)	0.0546 (5)
C16	0.71761 (17)	0.88929 (16)	0.46778 (13)	0.0460 (4)
C17	0.6199 (2)	0.24568 (18)	−0.05984 (14)	0.0588 (5)
C18	0.6905 (2)	0.1002 (2)	−0.04024 (18)	0.0698 (6)
C19	0.62085 (18)	0.25958 (16)	0.27124 (12)	0.0480 (4)
H1	0.06320	0.42360	0.13920	0.0680*
H2	0.05790	0.29130	−0.07200	0.0830*
H3	0.30130	0.21850	−0.15920	0.0760*
H6	0.719 (2)	0.3929 (18)	0.1796 (15)	0.048 (4)*
H7	0.48020	0.64840	0.46030	0.0470*

H8	0.23020	0.53570	0.35490	0.0510*
H12	0.97530	0.70250	0.59520	0.0620*
H13	1.02580	0.95050	0.74470	0.0730*
H14	0.88970	1.16000	0.71830	0.0690*
H15	0.69800	1.12250	0.54600	0.0650*
H16	0.63780	0.87410	0.39930	0.0550*
H17A	0.70600	0.33330	−0.02750	0.0710*
H17B	0.59700	0.22620	−0.14940	0.0710*
H18A	0.71600	0.11820	0.04800	0.1050*
H18B	0.79130	0.07950	−0.08100	0.1050*
H18C	0.60870	0.01100	−0.07530	0.1050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0357 (5)	0.0583 (6)	0.0750 (7)	0.0123 (4)	0.0035 (5)	−0.0035 (5)
N1	0.0335 (5)	0.0385 (5)	0.0388 (5)	0.0050 (4)	0.0048 (4)	0.0046 (4)
N2	0.0948 (11)	0.0607 (8)	0.0668 (9)	0.0215 (8)	−0.0015 (8)	0.0277 (7)
C1	0.0426 (7)	0.0596 (9)	0.0638 (9)	0.0006 (6)	−0.0058 (6)	0.0162 (7)
C2	0.0592 (10)	0.0764 (11)	0.0620 (10)	−0.0044 (8)	−0.0192 (8)	0.0179 (8)
C3	0.0801 (11)	0.0634 (9)	0.0387 (7)	−0.0084 (8)	−0.0084 (7)	0.0116 (6)
C4	0.0628 (9)	0.0406 (6)	0.0394 (6)	−0.0031 (6)	0.0047 (6)	0.0126 (5)
C5	0.0436 (6)	0.0347 (6)	0.0384 (6)	0.0000 (5)	0.0026 (5)	0.0125 (5)
C6	0.0373 (6)	0.0392 (6)	0.0394 (6)	0.0067 (5)	0.0074 (5)	0.0062 (5)
C7	0.0378 (6)	0.0392 (6)	0.0396 (6)	0.0078 (5)	0.0086 (5)	0.0086 (5)
C8	0.0347 (6)	0.0441 (7)	0.0487 (7)	0.0059 (5)	0.0089 (5)	0.0129 (5)
C9	0.0396 (6)	0.0395 (6)	0.0468 (7)	0.0003 (5)	−0.0001 (5)	0.0151 (5)
C10	0.0339 (6)	0.0416 (6)	0.0467 (7)	0.0068 (5)	0.0041 (5)	0.0102 (5)
C11	0.0326 (6)	0.0402 (6)	0.0423 (6)	0.0016 (5)	0.0044 (5)	0.0107 (5)
C12	0.0424 (7)	0.0521 (8)	0.0562 (8)	0.0076 (6)	−0.0046 (6)	0.0140 (6)
C13	0.0528 (8)	0.0674 (10)	0.0496 (8)	0.0018 (7)	−0.0100 (6)	0.0051 (7)
C14	0.0619 (9)	0.0471 (7)	0.0512 (8)	−0.0019 (6)	0.0060 (7)	−0.0007 (6)
C15	0.0657 (9)	0.0417 (7)	0.0552 (8)	0.0108 (6)	0.0076 (7)	0.0127 (6)
C16	0.0493 (7)	0.0448 (7)	0.0423 (7)	0.0080 (5)	0.0011 (5)	0.0123 (5)
C17	0.0764 (10)	0.0545 (8)	0.0418 (7)	−0.0044 (7)	0.0193 (7)	0.0085 (6)
C18	0.0783 (11)	0.0580 (9)	0.0704 (10)	0.0076 (8)	0.0327 (9)	0.0105 (8)
C19	0.0515 (8)	0.0451 (7)	0.0420 (7)	0.0140 (6)	−0.0013 (5)	0.0065 (5)

Geometric parameters (Å, °)

O1—C10	1.2161 (16)	C13—C14	1.376 (2)
N1—C6	1.4644 (16)	C14—C15	1.371 (2)
N1—C7	1.4086 (16)	C15—C16	1.381 (2)
N1—C10	1.3830 (16)	C17—C18	1.517 (3)
N2—C19	1.136 (2)	C1—H1	0.9297
C1—C2	1.372 (2)	C2—H2	0.9295
C1—C9	1.395 (2)	C3—H3	0.9295
C2—C3	1.376 (2)	C6—H6	0.952 (16)
C3—C4	1.402 (2)	C7—H7	0.9297

C4—C5	1.3966 (18)	C8—H8	0.9298
C4—C17	1.508 (2)	C12—H12	0.9297
C5—C6	1.5150 (18)	C13—H13	0.9297
C5—C9	1.3998 (18)	C14—H14	0.9295
C6—C19	1.488 (2)	C15—H15	0.9304
C7—C8	1.3298 (18)	C16—H16	0.9298
C8—C9	1.4577 (18)	C17—H17A	0.9697
C10—C11	1.4875 (18)	C17—H17B	0.9699
C11—C12	1.3909 (19)	C18—H18A	0.9599
C11—C16	1.384 (2)	C18—H18B	0.9595
C12—C13	1.382 (2)	C18—H18C	0.9601
O1···C8^{i}	3.4083 (17)	C19···H18C^{x}	3.0932
O1···C19	3.1458 (19)	H1···O1^{v}	2.6766
O1···H1^{i}	2.6766	H1···H8	2.5458
O1···H6	2.297 (16)	H2···H14^{xi}	2.5152
O1···H8^{i}	2.5682	H3···H17B	2.3539
O1···H12	2.7188	H6···O1	2.297 (16)
O1···H12^{ii}	2.6267	H6···C17	2.635 (16)
N2···C15^{iii}	3.401 (2)	H6···C18	2.965 (17)
N1···H16	2.8139	H6···H17A	2.2203
N2···H15^{iii}	2.8074	H6···H18A	2.4331
N2···H7^{iv}	2.8264	H7···C11	2.6808
C6···C18	3.375 (2)	H7···C16	2.7713
C7···C7^{iv}	3.4726 (19)	H7···N2^{iv}	2.8264
C7···C16	3.124 (2)	H7···C19^{iv}	3.0707
C8···C19	3.337 (2)	H7···H15^{viii}	2.5735
C8···O1^{v}	3.4083 (17)	H8···O1^{v}	2.5682
C15···N2^{vi}	3.401 (2)	H8···H1	2.5458
C16···C7	3.124 (2)	H12···O1	2.7188
C18···C19	3.458 (2)	H12···O1^{ii}	2.6267
C18···C6	3.375 (2)	H14···H2^{xii}	2.5152
C19···C8	3.337 (2)	H15···N2^{vi}	2.8074
C19···O1	3.1458 (19)	H15···C7^{viii}	2.9866
C19···C18	3.458 (2)	H15···H7^{viii}	2.5735
C1···H17A^{vii}	3.0312	H16···N1	2.8139
C5···H18A	3.0963	H16···C7	2.8058
C6···H18A	2.8026	H17A···C6	2.8270
C6···H17A	2.8270	H17A···H6	2.2203
C7···H16	2.8058	H17A···C1^{vii}	3.0312
C7···H15^{viii}	2.9866	H17B···H3	2.3539
C11···H7	2.6808	H18A···C5	3.0963
C13···H18B^{ix}	3.0669	H18A···C6	2.8026
C14···H18B^{ix}	3.0034	H18A···C19	2.6346
C16···H7	2.7713	H18A···H6	2.4331

C17···H6	2.635 (16)	H18B···C13^{xiii}	3.0669
C18···H6	2.965 (17)	H18B···C14^{xiii}	3.0034
C18···H18C^{x}	3.0853	H18C···C18^{x}	3.0853
C19···H18A	2.6346	H18C···C19^{x}	3.0932
C19···H7^{iv}	3.0707	H18C···H18C^{x}	2.5755
C6—N1—C7	116.28 (10)	C9—C1—H1	120.15
C6—N1—C10	116.35 (10)	C1—C2—H2	119.61
C7—N1—C10	124.71 (10)	C3—C2—H2	119.63
C2—C1—C9	119.75 (14)	C2—C3—H3	119.14
C1—C2—C3	120.75 (15)	C4—C3—H3	119.12
C2—C3—C4	121.73 (14)	N1—C6—H6	108.1 (10)
C3—C4—C5	116.80 (13)	C5—C6—H6	112.1 (10)
C3—C4—C17	120.35 (12)	C19—C6—H6	106.7 (10)
C5—C4—C17	122.84 (13)	N1—C7—H7	119.58
C4—C5—C6	121.65 (12)	C8—C7—H7	119.57
C4—C5—C9	121.83 (12)	C7—C8—H8	119.44
C6—C5—C9	116.42 (11)	C9—C8—H8	119.43
N1—C6—C5	111.72 (10)	C11—C12—H12	120.17
N1—C6—C19	108.87 (10)	C13—C12—H12	120.22
C5—C6—C19	109.26 (11)	C12—C13—H13	119.88
N1—C7—C8	120.86 (12)	C14—C13—H13	119.87
C7—C8—C9	121.13 (12)	C13—C14—H14	119.95
C1—C9—C5	119.06 (12)	C15—C14—H14	119.92
C1—C9—C8	122.04 (12)	C14—C15—H15	119.79
C5—C9—C8	118.72 (11)	C16—C15—H15	119.78
O1—C10—N1	119.64 (12)	C11—C16—H16	120.13
O1—C10—C11	121.78 (12)	C15—C16—H16	120.09
N1—C10—C11	118.56 (11)	C4—C17—H17A	108.32
C10—C11—C12	117.94 (12)	C4—C17—H17B	108.33
C10—C11—C16	121.96 (11)	C18—C17—H17A	108.28
C12—C11—C16	119.77 (12)	C18—C17—H17B	108.29
C11—C12—C13	119.61 (14)	H17A—C17—H17B	107.42
C12—C13—C14	120.26 (15)	C17—C18—H18A	109.43
C13—C14—C15	120.14 (15)	C17—C18—H18B	109.46
C14—C15—C16	120.43 (15)	C17—C18—H18C	109.43
C11—C16—C15	119.78 (13)	H18A—C18—H18B	109.50
C4—C17—C18	115.89 (13)	H18A—C18—H18C	109.50
N2—C19—C6	177.79 (16)	H18B—C18—H18C	109.51
C2—C1—H1	120.10		
C7—N1—C6—C5	43.48 (14)	C4—C5—C9—C8	−172.67 (13)
C7—N1—C6—C19	−77.28 (14)	C6—C5—C9—C1	−173.80 (13)
C10—N1—C6—C5	−154.13 (11)	C6—C5—C9—C8	10.84 (19)
C10—N1—C6—C19	85.12 (14)	C4—C5—C6—C19	−93.33 (15)
C6—N1—C7—C8	−22.81 (18)	C9—C5—C6—N1	−37.36 (16)
C10—N1—C7—C8	176.44 (13)	C9—C5—C6—C19	83.17 (14)
C6—N1—C10—O1	−2.57 (18)	C4—C5—C9—C1	2.7 (2)
C6—N1—C10—C11	175.59 (11)	N1—C7—C8—C9	−6.4 (2)

C7—N1—C10—O1	158.17 (13)	C7—C8—C9—C5	12.3 (2)
C7—N1—C10—C11	−23.67 (19)	C7—C8—C9—C1	−162.93 (15)
C2—C1—C9—C5	−1.1 (2)	O1—C10—C11—C16	132.02 (15)
C2—C1—C9—C8	174.15 (15)	N1—C10—C11—C12	140.61 (13)
C9—C1—C2—C3	−1.2 (3)	N1—C10—C11—C16	−46.10 (18)
C1—C2—C3—C4	1.9 (3)	O1—C10—C11—C12	−41.28 (19)
C2—C3—C4—C17	−179.25 (16)	C10—C11—C12—C13	173.43 (13)
C2—C3—C4—C5	−0.3 (2)	C16—C11—C12—C13	0.0 (2)
C17—C4—C5—C9	176.92 (14)	C10—C11—C16—C15	−171.86 (13)
C17—C4—C5—C6	−6.8 (2)	C12—C11—C16—C15	1.3 (2)
C3—C4—C5—C6	174.32 (13)	C11—C12—C13—C14	−1.1 (2)
C3—C4—C17—C18	−105.68 (17)	C12—C13—C14—C15	0.9 (2)
C5—C4—C17—C18	75.46 (19)	C13—C14—C15—C16	0.4 (2)
C3—C4—C5—C9	−2.0 (2)	C14—C15—C16—C11	−1.5 (2)
C4—C5—C6—N1	146.14 (12)		

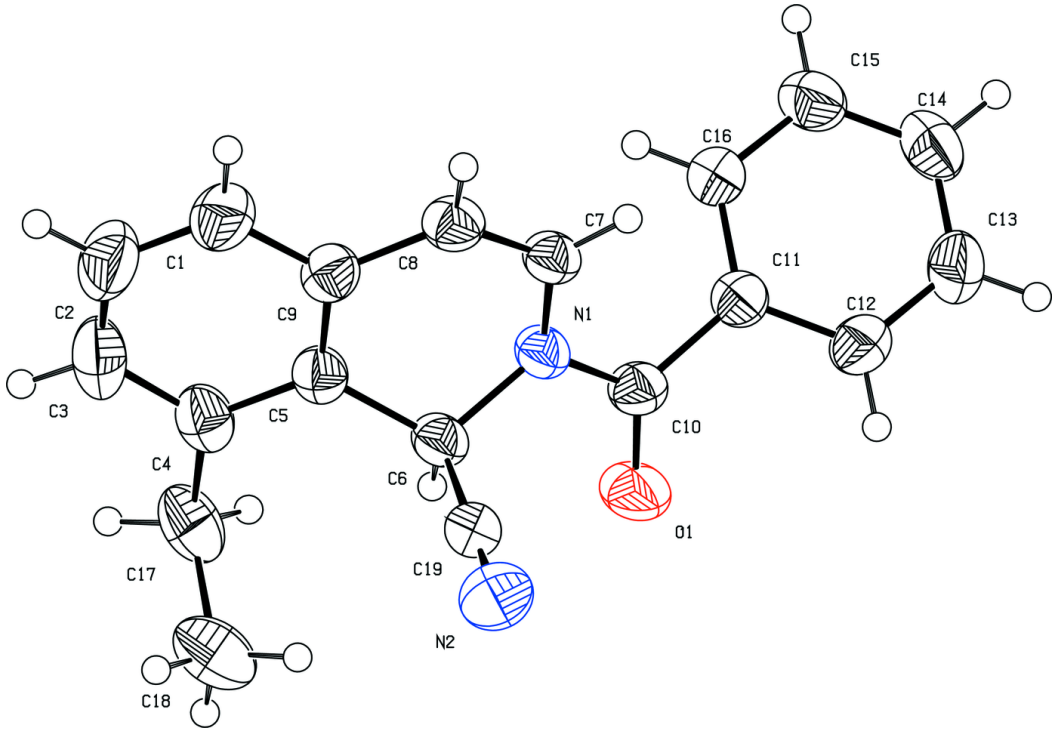
Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*−1, *y*, *z*; (vi) *x*, *y*+1, *z*; (vii) −*x*+1, −*y*+1, −*z*; (viii) −*x*+1, −*y*+2, −*z*+1; (ix) *x*, *y*+1, *z*+1; (x) −*x*+1, −*y*, −*z*; (xi) *x*−1, *y*−1, *z*−1; (xii) *x*+1, *y*+1, *z*+1; (xiii) *x*, *y*−1, *z*−1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1	0.952 (16)	2.297 (16)	2.6471 (17)	100.9 (11)
C8—H8···O1^{v}	0.93	2.57	3.4083 (17)	151

Symmetry codes: (v) *x*−1, *y*, *z*.

Fig. 1


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