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(*Z*)-4-[3-(2,5-Dioxoimidazolidin-4-ylidenemethyl)-1*H*-indol-1-ylmethyl]benzonitrile

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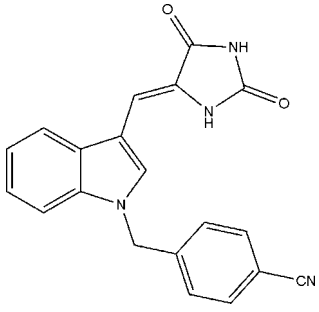
Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.088; data-to-parameter ratio = 12.8.

In the title compound, $C_{20}H_{14}N_4O_2$, molecules are linked into chains by N—H···O hydrogen bonds, but the cyano group does not participate in the supramolecular aggregation. The crystal structure of the compound indicates the presence of a double bond with *Z* geometry, connecting the imidazolidine and indole units. The dihedral angle between the imidazole and benzene ring planes is 62.45 (4)°.

Related literature

For 2-indol-3-yl-methylenequinuclidin-3-ols NADPH oxidase activity, see: Sekhar *et al.* (2003). For novel substituted (*Z*)-2-(*N*-benzylindol-3-ylmethylene)quinuclidin-3-one and (*Z*)-(±)-2-(*N*-benzylindol-3-ylmethylene)quinuclidin-3-ol derivatives as potent thermal sensitizing agents, see: Sonar *et al.* (2007). For the molecular structures of di- and triindolylmethanes, see: Mason *et al.* (2003). For the structures of 1*H*-indole-3-ethylene-3′-methoxysalicylaldimine and 3-[3′-azapentyl-3′-en-4′-(2′′-hydroxyphenyl)]indole, see: Zarza *et al.* (1988).



Experimental

Crystal data

$C_{20}H_{14}N_4O_2$
M_r = 342.35
Monoclinic, $C2/c$
a = 18.8495 (16) Å
b = 7.6812 (7) Å
c = 24.322 (2) Å
β = 110.939 (3)°
V = 3289.0 (5) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.76 mm^{-1}
T = 90.0 (2) K
0.15 × 0.08 × 0.06 mm

Data collection

Bruker X8 Proteum diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.806, T_{max} = 0.957
23493 measured reflections
3025 independent reflections
2849 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.088
S = 1.04
3025 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^{i}	0.88	1.95	2.8237 (12)	173
N4—H4···O2^{ii}	0.88	2.07	2.8740 (13)	151

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and local procedures.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2156).

References

Bruker (2006). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc, Madison, Wisconsin, USA.
Mason, M. R., Barnard, T. S., Segla, M. F., Xie, B. & Kirschbaum, K. (2003). *J. Chem. Crystallogr.* **33**, 531–540.
Sekhar, K. R., Crooks, P. A., Sonar, V. N., Friedman, D. B., Chan, J. Y., Meredith, M. J., Stames, J. H., Kelton, K. R., Summar, S. R., Sasi, S. & Freeman, M. L. (2003). *Cancer Res.* **63**, 5636–5645.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sonar, V. N., Reddy, Y. T., Sekhar, K. R., Sowmya, S., Freeman, M. L. & Crooks, P. A. (2007). *Bioorg. Med. Chem. Lett.* **17**, 6821–6824.
Zarza, P. M., Gill, P., Díaz González, M. C., Martin Reyes, M. G., Arrieta, J. M., Nastopoulos, V., Germain, G. & Debaerdemaeker, T. (1988). *Acta Cryst.* C**44**, 678–681.

supplementary materials

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(*Z*)-4-[3-(2,5-Dioxoimidazolidin-4-ylidenemethyl)-1*H*-indol-1-ylmethyl]benzonitrile

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Comment

As part of a continuing search for biologically active molecules containing indole ring systems (Sonar *et al.*, 2007), we have now prepared the title compound by the reaction of 4-(3-formyl-1*H*-indol-1-ylmethyl)benzonitrile with imidazolidine-2,4-dione in the presence of ammonium acetate in acetic acid at 393 K. The compound was crystallized from a mixture of methanol and ethylacetate. The molecular structure and the atom-numbering scheme are shown in Fig.1. The indole ring is planar with bond distances and angles comparable with those previously reported for other indole derivatives (Mason *et al.*, 2003; Zarza, *et al.*, 1988). The X-ray studies revealed that the obtained compound is the *Z* isomer. The C18—C19 bond is in a *trans* position with respect to the C2—C17 bond. The olefinic bond (C17=C18) has a planar atomic arrangement, since the r.m.s. deviation from the mean plane passing through atoms C2, C17, C18, N4 is 0.0009 (5) Å. The maximum deviation from plane for imidazoline ring is 0.0087 Å. Deviations from ideal geometry are observed in the bond angles around atoms C2, C17 and C18. The C17=C18—C19 bond angle is close to the standard planar triangular value of 120°, whereas the C1=C2—C17, C18—C17=C2 and C17=C18—N4 bond angles are more distorted due to the strain induced by the C17=C18—C1=O1 conjugated double bond linkage. These bond angle deformations, which require little energy, are needed to release the intramolecular interactions between non-bonded atoms. The imidazolidine ring, which makes a dihedral angle of 2.48 (5)° with the adjacent aromatic ring presents very small distortions around atoms N4, C20, N3 and C19.

Significant intermolecular hydrogen-bonding interactions are found between N(3)—H(3)···O(1) and N(4)—H(4)···O(2). Molecules are linked into chains by a series of N—H···O hydrogen bonds.

Experimental

A mixture of 4-(3-formyl-indol-1-ylmethyl)benzonitrile (0.5 g, 1.92 mmol), imidazolidine-2,4-dione (0.23 g, 2.30 mmol) and ammonium acetate (0.15 g, 1.94 mmol) was stirred in acetic acid (5 ml) at 393 K for 10 hrs. The reaction mixture was cooled to room temperature and the yellow solid that separated was collected by filtration, washed with cold water and dried to afford the the crude product. Crystallization from methanol and ethyl acetate (1:1) gave a yellow crystalline product of (*Z*)-4-((3-((2,5- dioxoimidazolidin-4-ylidene)methyl)-1*H*-indol-1-yl)methyl) benzonitrile that was suitable for X-ray analysis. ^{1}H NMR (DMSO d_6): δ 5.56 (*s*, 2H), 6.7 (*s*, 1H), 7.13–7.23 (*m*, 2H), 7.44–7.53 (*m*, 3H), 7.79–7.83 (*m*, 3H), 8.30 (*s*, 1H), 10.15 (*bs*, 1H), 11.07 (*bs*, 1H); ^{13}C NMR (DMSO d_6): δ 101.46, 109.25, 111.06, 111.22, 119.21, 119.29, 121.34, 123.42, 124.95, 128.10, 128.70, 130.63, 133.26, 136.25, 143.71, 155.94, 165.87.

Refinement

H atoms were found in difference Fourier maps and subsequently placed in idealized positions with constrained distances of 0.99 Å (R_2CH_2), 0.95 Å (R_2CH) and 0.88 Å (NH) with U_{iso}(H) values set to 1.2U_{eq} of the attached atom.

Figures

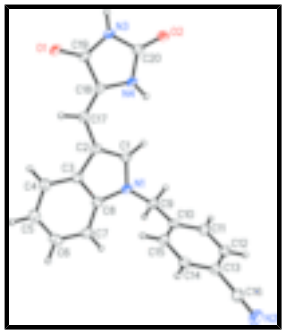


Fig. 1. A view of the molecule with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

(*Z*)-4-[3-(2,5-Dioxoimidazolidin-4-ylidenemethyl)-1*H*-indol- 1-ylmethyl]benzonitrile

Crystal data

$C_{20}H_{14}N_4O_2$	F_{000} = 1424
M_r = 342.35	D_x = 1.383 Mg m^{-3}
Monoclinic, *C*2/*c*	Cu *K*α radiation λ = 1.54178 Å
Hall symbol: -C 2yc	Cell parameters from 9981 reflections
a = 18.8495 (16) Å	θ = 3.9–68.8º
b = 7.6812 (7) Å	μ = 0.76 mm^{-1}
c = 24.322 (2) Å	*T* = 90.0 (2) K
β = 110.939 (3)º	Block, yellow
V = 3289.0 (5) Å^3	0.15 × 0.08 × 0.06 mm
Z = 8	

Data collection

Bruker X8 Proteum diffractometer	3025 independent reflections
Radiation source: fine-focus rotating anode	2849 reflections with $I > 2\sigma(I)$
Monochromator: graded multilayer optics	R_{int} = 0.039
Detector resolution: 18 pixels mm^{-1}	θ_{max} = 68.8º
T = 90.0(2) K	θ_{min} = 3.9º
φ and ω scans	*h* = −22→22
Absorption correction: multi-scan (SADABS in APEX2; Bruker, 2006)	*k* = −9→9
T_{min} = 0.806, T_{max} = 0.957	*l* = −28→29
23493 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.088$

$S = 1.04$

3025 reflections

236 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 2.7005P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.24$ e Å^{-3}

$\Delta\rho_{min} = -0.30$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00030 (6)

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}
N1	0.41106 (5)	0.49108 (13)	0.60476 (4)	0.0204 (2)
N2	0.28685 (7)	0.12998 (16)	0.84996 (5)	0.0344 (3)
N3	0.66684 (5)	0.16845 (13)	0.50768 (4)	0.0204 (2)
H3	0.7010	0.1248	0.4946	0.024*
N4	0.56545 (5)	0.18829 (13)	0.53212 (4)	0.0213 (2)
H4	0.5232	0.1612	0.5377	0.026*
O1	0.71827 (4)	0.44259 (11)	0.53352 (4)	0.0233 (2)
O2	0.58759 (5)	−0.07063 (12)	0.49259 (4)	0.0300 (2)
C1	0.46081 (6)	0.41065 (15)	0.58406 (5)	0.0196 (2)
H1	0.4549	0.2960	0.5684	0.024*
C2	0.52091 (6)	0.51930 (15)	0.58903 (5)	0.0185 (2)
C3	0.50688 (6)	0.67773 (15)	0.61526 (5)	0.0201 (2)
C4	0.54595 (7)	0.83512 (16)	0.63133 (6)	0.0269 (3)
H4A	0.5928	0.8535	0.6257	0.032*
C5	0.51500 (8)	0.96293 (17)	0.65546 (7)	0.0343 (3)
H5	0.5412	1.0703	0.6668	0.041*
C6	0.44596 (8)	0.93872 (17)	0.66367 (6)	0.0337 (3)
H6	0.4263	1.0298	0.6805	0.040*
C7	0.40588 (7)	0.78571 (17)	0.64794 (6)	0.0271 (3)
H7	0.3587	0.7693	0.6531	0.033*
C8	0.43762 (6)	0.65602 (15)	0.62406 (5)	0.0210 (3)
C9	0.33815 (6)	0.41858 (17)	0.60065 (5)	0.0235 (3)

H9A	0.3245	0.3259	0.5704	0.028*
H9B	0.2993	0.5112	0.5869	0.028*
C10	0.33468 (6)	0.34369 (15)	0.65670 (5)	0.0199 (3)
C11	0.27885 (7)	0.22088 (16)	0.65210 (5)	0.0245 (3)
H11	0.2487	0.1771	0.6145	0.029*
C12	0.26669 (7)	0.16176 (16)	0.70142 (6)	0.0264 (3)
H12	0.2280	0.0786	0.6979	0.032*
C13	0.31168 (7)	0.22512 (15)	0.75657 (5)	0.0225 (3)
C14	0.36964 (7)	0.34280 (15)	0.76188 (5)	0.0222 (3)
H14	0.4013	0.3830	0.7996	0.027*
C15	0.38107 (6)	0.40105 (15)	0.71200 (5)	0.0216 (3)
H15	0.4209	0.4809	0.7155	0.026*
C16	0.29783 (7)	0.17006 (16)	0.80831 (5)	0.0266 (3)
C17	0.58384 (6)	0.49104 (15)	0.57005 (5)	0.0194 (2)
H17	0.6177	0.5866	0.5755	0.023*
C18	0.60159 (6)	0.34914 (15)	0.54582 (5)	0.0186 (2)
C19	0.66927 (6)	0.33333 (15)	0.52922 (5)	0.0190 (2)
C20	0.60397 (6)	0.07873 (16)	0.50901 (5)	0.0220 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0187 (5)	0.0246 (5)	0.0217 (5)	−0.0014 (4)	0.0117 (4)	−0.0015 (4)
N2	0.0372 (6)	0.0407 (7)	0.0285 (6)	−0.0136 (5)	0.0156 (5)	−0.0019 (5)
N3	0.0167 (5)	0.0266 (5)	0.0216 (5)	−0.0027 (4)	0.0116 (4)	−0.0056 (4)
N4	0.0171 (5)	0.0257 (5)	0.0260 (5)	−0.0045 (4)	0.0137 (4)	−0.0056 (4)
O1	0.0205 (4)	0.0268 (4)	0.0277 (4)	−0.0048 (3)	0.0148 (3)	−0.0036 (3)
O2	0.0242 (4)	0.0301 (5)	0.0419 (5)	−0.0081 (4)	0.0195 (4)	−0.0151 (4)
C1	0.0207 (5)	0.0222 (6)	0.0190 (5)	0.0000 (4)	0.0109 (4)	−0.0021 (4)
C2	0.0182 (5)	0.0215 (6)	0.0168 (5)	0.0010 (4)	0.0076 (4)	0.0007 (4)
C3	0.0206 (6)	0.0215 (6)	0.0198 (5)	0.0015 (4)	0.0091 (4)	0.0025 (4)
C4	0.0268 (6)	0.0223 (6)	0.0354 (7)	−0.0011 (5)	0.0156 (5)	0.0008 (5)
C5	0.0384 (7)	0.0207 (6)	0.0477 (8)	−0.0023 (5)	0.0201 (6)	−0.0046 (6)
C6	0.0387 (8)	0.0240 (7)	0.0440 (8)	0.0065 (5)	0.0215 (6)	−0.0037 (6)
C7	0.0270 (6)	0.0275 (6)	0.0318 (7)	0.0052 (5)	0.0166 (5)	0.0017 (5)
C8	0.0217 (6)	0.0218 (6)	0.0213 (6)	0.0019 (4)	0.0100 (5)	0.0022 (4)
C9	0.0181 (5)	0.0327 (7)	0.0223 (6)	−0.0031 (5)	0.0104 (5)	−0.0015 (5)
C10	0.0180 (5)	0.0214 (6)	0.0237 (6)	0.0021 (4)	0.0115 (5)	−0.0017 (4)
C11	0.0230 (6)	0.0280 (6)	0.0239 (6)	−0.0048 (5)	0.0102 (5)	−0.0050 (5)
C12	0.0255 (6)	0.0272 (6)	0.0296 (6)	−0.0080 (5)	0.0137 (5)	−0.0026 (5)
C13	0.0242 (6)	0.0225 (6)	0.0242 (6)	0.0004 (5)	0.0128 (5)	0.0012 (5)
C14	0.0228 (6)	0.0219 (6)	0.0222 (6)	−0.0005 (4)	0.0083 (5)	−0.0016 (4)
C15	0.0192 (5)	0.0216 (6)	0.0255 (6)	−0.0021 (4)	0.0100 (5)	−0.0005 (5)
C16	0.0270 (6)	0.0277 (6)	0.0267 (6)	−0.0060 (5)	0.0118 (5)	−0.0018 (5)
C17	0.0174 (5)	0.0234 (6)	0.0190 (5)	−0.0025 (4)	0.0083 (4)	0.0006 (4)
C18	0.0163 (5)	0.0238 (6)	0.0171 (5)	−0.0012 (4)	0.0078 (4)	0.0002 (4)
C19	0.0180 (5)	0.0252 (6)	0.0156 (5)	−0.0013 (4)	0.0081 (4)	−0.0006 (4)
C20	0.0186 (5)	0.0275 (6)	0.0225 (6)	−0.0038 (5)	0.0105 (4)	−0.0061 (5)

Geometric parameters (Å, °)

N1—C1	1.3608 (15)	C6—C7	1.3754 (19)
N1—C8	1.3815 (15)	C6—H6	0.9500
N1—C9	1.4527 (14)	C7—C8	1.3913 (17)
N2—C16	1.1459 (17)	C7—H7	0.9500
N3—C19	1.3650 (15)	C9—C10	1.5025 (16)
N3—C20	1.3812 (15)	C9—H9A	0.9900
N3—H3	0.8800	C9—H9B	0.9900
N4—C20	1.3576 (15)	C10—C11	1.3877 (17)
N4—C18	1.3926 (15)	C10—C15	1.3883 (16)
N4—H4	0.8800	C11—C12	1.3761 (17)
O1—C19	1.2246 (14)	C11—H11	0.9500
O2—C20	1.2178 (15)	C12—C13	1.3938 (17)
C1—C2	1.3772 (16)	C12—H12	0.9500
C1—H1	0.9500	C13—C14	1.3879 (17)
C2—C17	1.4348 (16)	C13—C16	1.4372 (17)
C2—C3	1.4416 (16)	C14—C15	1.3805 (17)
C3—C4	1.3967 (17)	C14—H14	0.9500
C3—C8	1.4064 (16)	C15—H15	0.9500
C4—C5	1.3759 (19)	C17—C18	1.3372 (17)
C4—H4A	0.9500	C17—H17	0.9500
C5—C6	1.398 (2)	C18—C19	1.4742 (15)
C5—H5	0.9500		
C1—N1—C8	109.16 (9)	C10—C9—H9A	108.4
C1—N1—C9	124.09 (10)	N1—C9—H9B	108.4
C8—N1—C9	126.44 (10)	C10—C9—H9B	108.4
C19—N3—C20	111.43 (9)	H9A—C9—H9B	107.5
C19—N3—H3	124.3	C11—C10—C15	119.39 (11)
C20—N3—H3	124.3	C11—C10—C9	117.71 (10)
C20—N4—C18	111.14 (9)	C15—C10—C9	122.75 (10)
C20—N4—H4	124.4	C12—C11—C10	120.79 (11)
C18—N4—H4	124.4	C12—C11—H11	119.6
N1—C1—C2	110.27 (10)	C10—C11—H11	119.6
N1—C1—H1	124.9	C11—C12—C13	119.35 (11)
C2—C1—H1	124.9	C11—C12—H12	120.3
C1—C2—C17	128.96 (11)	C13—C12—H12	120.3
C1—C2—C3	105.97 (10)	C14—C13—C12	120.33 (11)
C17—C2—C3	125.00 (10)	C14—C13—C16	119.57 (11)
C4—C3—C8	119.03 (11)	C12—C13—C16	120.10 (11)
C4—C3—C2	133.85 (11)	C15—C14—C13	119.62 (11)
C8—C3—C2	107.12 (10)	C15—C14—H14	120.2
C5—C4—C3	118.39 (12)	C13—C14—H14	120.2
C5—C4—H4A	120.8	C14—C15—C10	120.43 (11)
C3—C4—H4A	120.8	C14—C15—H15	119.8
C4—C5—C6	121.63 (13)	C10—C15—H15	119.8
C4—C5—H5	119.2	N2—C16—C13	178.46 (14)
C6—C5—H5	119.2	C18—C17—C2	129.12 (11)

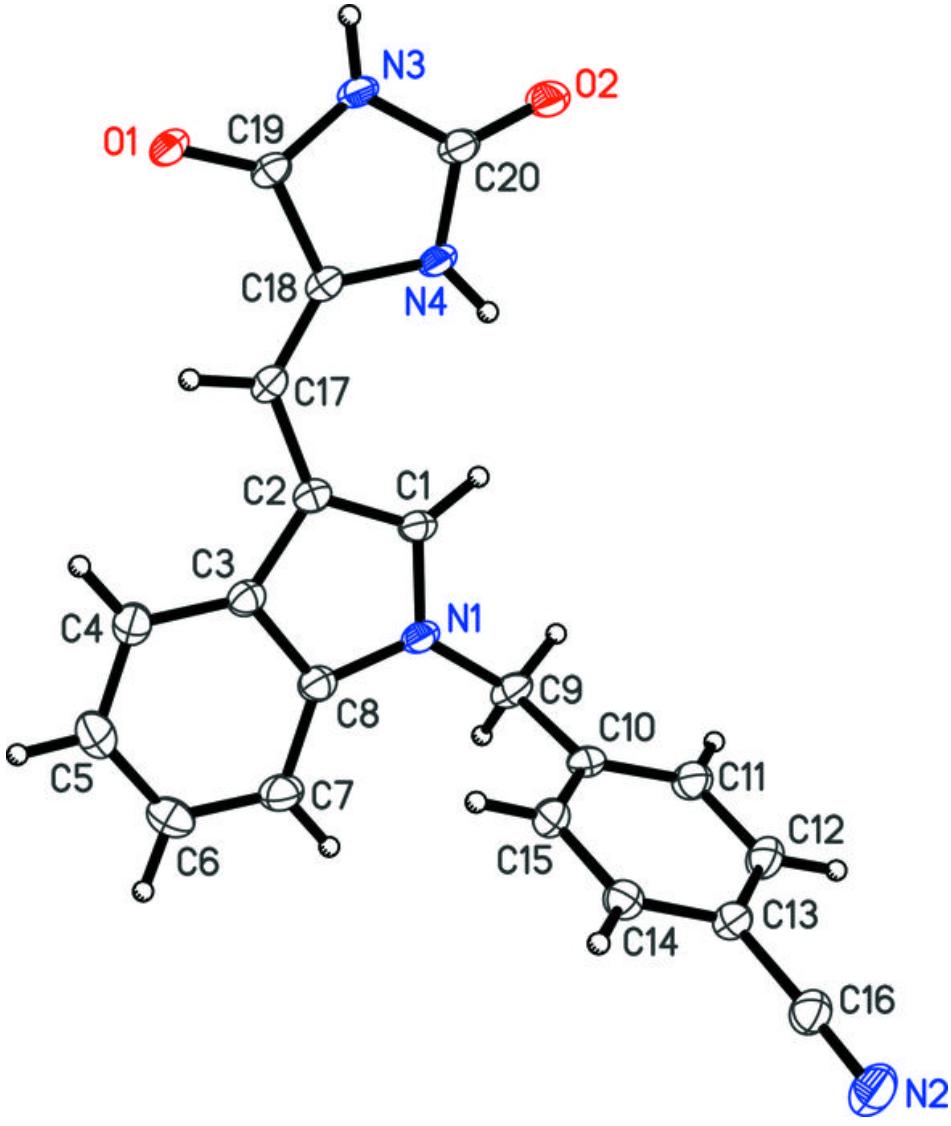
C7—C6—C5	121.37 (12)	C18—C17—H17	115.4
C7—C6—H6	119.3	C2—C17—H17	115.4
C5—C6—H6	119.3	C17—C18—N4	130.58 (10)
C6—C7—C8	116.92 (11)	C17—C18—C19	124.41 (10)
C6—C7—H7	121.5	N4—C18—C19	104.99 (9)
C8—C7—H7	121.5	O1—C19—N3	126.12 (10)
N1—C8—C7	129.86 (11)	O1—C19—C18	128.34 (10)
N1—C8—C3	107.48 (10)	N3—C19—C18	105.54 (9)
C7—C8—C3	122.66 (11)	O2—C20—N4	127.55 (11)
N1—C9—C10	115.55 (9)	O2—C20—N3	125.55 (11)
N1—C9—H9A	108.4	N4—C20—N3	106.90 (10)
C8—N1—C1—C2	−0.07 (13)	C15—C10—C11—C12	3.09 (18)
C9—N1—C1—C2	173.86 (10)	C9—C10—C11—C12	−172.46 (11)
N1—C1—C2—C17	−176.56 (11)	C10—C11—C12—C13	−0.67 (19)
N1—C1—C2—C3	0.49 (13)	C11—C12—C13—C14	−1.89 (19)
C1—C2—C3—C4	−179.90 (13)	C11—C12—C13—C16	177.54 (11)
C17—C2—C3—C4	−2.7 (2)	C12—C13—C14—C15	1.98 (18)
C1—C2—C3—C8	−0.72 (12)	C16—C13—C14—C15	−177.45 (11)
C17—C2—C3—C8	176.48 (10)	C13—C14—C15—C10	0.48 (17)
C8—C3—C4—C5	0.24 (18)	C11—C10—C15—C14	−2.99 (17)
C2—C3—C4—C5	179.34 (12)	C9—C10—C15—C14	172.32 (11)
C3—C4—C5—C6	−0.4 (2)	C1—C2—C17—C18	−4.0 (2)
C4—C5—C6—C7	0.0 (2)	C3—C2—C17—C18	179.49 (11)
C5—C6—C7—C8	0.6 (2)	C2—C17—C18—N4	−0.3 (2)
C1—N1—C8—C7	179.20 (12)	C2—C17—C18—C19	−178.46 (11)
C9—N1—C8—C7	5.45 (19)	C20—N4—C18—C17	−178.60 (12)
C1—N1—C8—C3	−0.40 (12)	C20—N4—C18—C19	−0.22 (12)
C9—N1—C8—C3	−174.15 (10)	C20—N3—C19—O1	179.92 (11)
C6—C7—C8—N1	179.66 (12)	C20—N3—C19—C18	0.11 (12)
C6—C7—C8—C3	−0.79 (18)	C17—C18—C19—O1	−1.22 (19)
C4—C3—C8—N1	−179.99 (10)	N4—C18—C19—O1	−179.74 (11)
C2—C3—C8—N1	0.69 (12)	C17—C18—C19—N3	178.58 (10)
C4—C3—C8—C7	0.38 (17)	N4—C18—C19—N3	0.06 (11)
C2—C3—C8—C7	−178.95 (11)	C18—N4—C20—O2	179.95 (12)
C1—N1—C9—C10	103.89 (13)	C18—N4—C20—N3	0.28 (13)
C8—N1—C9—C10	−83.24 (14)	C19—N3—C20—O2	−179.91 (11)
N1—C9—C10—C11	−157.33 (11)	C19—N3—C20—N4	−0.24 (13)
N1—C9—C10—C15	27.28 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1^{i}	0.88	1.95	2.8237 (12)	173
N4—H4···O2^{ii}	0.88	2.07	2.8740 (13)	151

Symmetry codes: (i) −*x*+3/2, −*y*+1/2, −*z*+1; (ii) −*x*+1, −*y*, −*z*+1.

Fig. 1


N3
O2
O1
C19
C20
C18
N4
C17
C2
C1
C3
C4
N1
C8
C9
C10
C11
C5
C7
C12
C15
C6
C13
C14
C16
N2