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2-(1*H*-Benzotriazol-1-yl)-1-(2-fluorobenzoyl)ethyl isonicotinate

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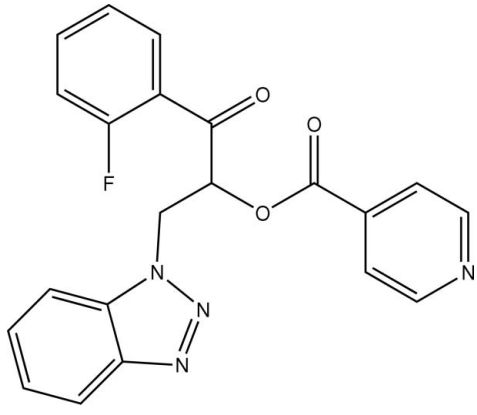
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.112; data-to-parameter ratio = 13.5.

The title compound, $C_{21}H_{15}FN_4O_3$, has a nonplanar conformation. The mean plane of the benzotriazole group makes dihedral angles of 79.30 (1) and 11.64 (1)° with the pyridine and benzene rings, respectively. An intramolecular C—H···F hydrogen bond forms a six-membered ring. Molecules are linked into dimers by C—H···O hydrogen bonds, and are linked into chains along the b axis by intermolecular C—H···N hydrogen bonds. The packing is further stabilized by weak π–π interactions with a distance of 3.752 (2) Å between the centroids of the benzene rings.

Related literature

For a related compound, see: Han *et al.* (2007). For related literature, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{15}FN_4O_3$
M_r = 390.37
Triclinic, $P\overline{1}$
a = 9.743 (4) Å
b = 10.226 (4) Å
c = 10.975 (4) Å
α = 99.167 (5)°
β = 114.399 (5)°
γ = 103.444 (5)°
V = 927.4 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.26 × 0.20 × 0.04 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.996
5185 measured reflections
3544 independent reflections
2651 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
S = 1.04
3544 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···N3^{i}	0.93	2.50	3.427 (3)	172
C8—H8A···F1	0.98	2.25	2.759 (2)	112
C15—H15A···O1^{ii}	0.93	2.54	3.452 (3)	168
C21—H21A···N2^{iii}	0.93	2.57	3.398 (3)	148

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+2, -z+2$; (iii) $-x+1, -y+1, -z+2$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2386).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Han, X.-J., Zeng, W.-L., Bi, S. & Wan, J. (2007). *Acta Cryst.* E**63**, o1194–o1195.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supplementary materials

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2-(1*H*-Benzotriazol-1-yl)-1-(2-fluorobenzoyl)ethyl isonicotinate

J. Wan, F. Li, W.-L. Zeng, J. Li and S. Bi

Comment

We have recently reported the structure of 2-(1*H*-benzotriazol-1-yl)-1-(4-chlorobenzoyl)ethyl isonicotinate (II) (Han *et al.*, 2007). As part of our ongoing studies of triazole derivatives, the title compound, (I), was synthesized and its structure is reported here.

All the bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable to those in the related compound (II). In (I), the benzotriazole system is essentially planar, with a dihedral angle of 1.89 (1)° between triazole ring A(N1—N3/C10/C11) and benzene ring B(C10—C15). The mean plane of the benzotriazole group makes dihedral angles 79.30 (1)° and 11.64 (1)° with the C(N4/C17—C21) and D(C1—C6) rings, respectively. The dihedral angle between the planes of the latter two aromatic rings is 76.08 (1)°. There is an intramolecular C8—H8A···F1 hydrogen bond, forming a six-membered ring.

In the crystal structure, molecules of (I) are linked into dimers by C15—H15A···O1^{ii} hydrogen bonds [symmetry code: (ii) $1-x, 2-y, 2-z$], and are linked into chains along the *b* axis by intermolecular C2—H2B···N3^{i} and C21—H21A···N2^{iii} [symmetry codes: (i) $1-x, 1-y, 1-z$; (iii) $1-x, 1-y, 2-z$] hydrogen bonds (Table 1 and Fig. 2). The packing is further stabilized by weak π-π interactions involving the C1—C6 benzene rings: *Cg*3···*Cg*3^{iv} = 3.752 Å [symmetry code: (iv) $-x, 1-y, 1-z$, *Cg*3 is the centroid of the C1—C6 benzene ring].

Experimental

The title compound (I) was prepared according to the literature method of Han *et al.* (2007). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of 6 days.

Refinement

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) H atoms.

Figures

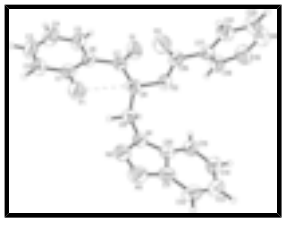

Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

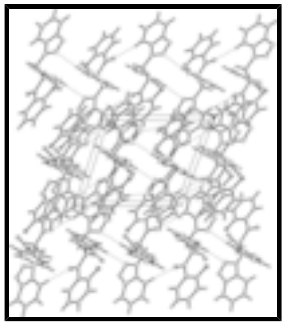

Fig. 2. A packing diagram of (I), viewed down the *c* axis. Hydrogen bonds are indicated by dashed lines.

2-(1*H*-Benzotriazol-1-yl)-1-(2-fluorobenzoyl)ethyl isonicotinate

Crystal data

$C_{21}H_{15}FN_4O_3$	$Z = 2$
$M_r = 390.37$	$F_{000} = 404$
Triclinic, $P\overline{1}$	$D_x = 1.398$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.743$ (4) Å	Cell parameters from 1764 reflections
$b = 10.226$ (4) Å	$\theta = 2.4$–25.1°
$c = 10.975$ (4) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 99.167$ (5)°	$T = 293$ (2) K
$\beta = 114.399$ (5)°	Plate, yellow
$\gamma = 103.444$ (5)°	0.26 × 0.20 × 0.04 mm
$V = 927.4$ (6) Å^3	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3544 independent reflections
Radiation source: fine-focus sealed tube	2651 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.015$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.0^\circ$
$T = 293(2)$ K	$\theta_{min} = 2.1^\circ$
ω scans	$h = -8 \rightarrow 11$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -11 \rightarrow 12$
$T_{min} = 0.974$, $T_{max} = 0.996$	$l = -13 \rightarrow 9$
5185 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained

$wR(F^2) = 0.112$	$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.134P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3544 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.18$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
F1	0.32317 (13)	0.57552 (11)	0.57280 (10)	0.0669 (3)
O2	0.53117 (13)	0.76959 (12)	0.99687 (11)	0.0488 (3)
O1	0.28064 (16)	0.84106 (14)	0.87200 (12)	0.0671 (4)
N1	0.72690 (16)	0.78363 (14)	0.85732 (14)	0.0471 (3)
C6	0.19491 (18)	0.72253 (16)	0.63796 (16)	0.0439 (4)
O3	0.35710 (17)	0.56942 (14)	0.97541 (13)	0.0697 (4)
C17	0.51604 (19)	0.73892 (17)	1.19893 (16)	0.0451 (4)
C16	0.45878 (19)	0.68059 (18)	1.04674 (17)	0.0464 (4)
C1	0.2037 (2)	0.63174 (17)	0.53563 (17)	0.0484 (4)
N2	0.72997 (18)	0.68140 (16)	0.76401 (15)	0.0615 (4)
C7	0.30749 (19)	0.76998 (17)	0.79067 (17)	0.0451 (4)
C10	0.86206 (19)	0.82372 (17)	0.98201 (17)	0.0460 (4)
C8	0.46330 (19)	0.73576 (17)	0.84731 (15)	0.0441 (4)
H8A	0.4426	0.6362	0.8070	0.053*
C9	0.58719 (19)	0.82737 (18)	0.81896 (17)	0.0483 (4)
H9A	0.5405	0.8219	0.7205	0.058*
H9B	0.6188	0.9243	0.8718	0.058*
C11	0.9478 (2)	0.73988 (19)	0.95988 (19)	0.0538 (4)
C2	0.0959 (2)	0.5924 (2)	0.39624 (18)	0.0606 (5)
H2B	0.1062	0.5311	0.3308	0.073*
N3	0.8622 (2)	0.65436 (18)	0.82430 (18)	0.0692 (5)
N4	0.5995 (2)	0.8432 (2)	1.48007 (17)	0.0724 (5)
C18	0.5974 (2)	0.87952 (19)	1.26949 (18)	0.0555 (5)
H18A	0.6272	0.9419	1.2247	0.067*
C5	0.0653 (2)	0.7722 (2)	0.59237 (19)	0.0598 (5)

H5A	0.0527	0.8316	0.6575	0.072*
C20	0.5256 (3)	0.7073 (2)	1.4117 (2)	0.0700 (6)
H20A	0.5036	0.6464	1.4609	0.084*
C21	0.4795 (2)	0.6509 (2)	1.2722 (2)	0.0596 (5)
H21A	0.4249	0.5554	1.2285	0.072*
C3	−0.0276 (2)	0.6459 (2)	0.3560 (2)	0.0694 (6)
H3B	−0.1011	0.6217	0.2619	0.083*
C19	0.6335 (3)	0.9256 (2)	1.4075 (2)	0.0688 (5)
H19A	0.6852	1.0212	1.4530	0.083*
C15	0.9200 (2)	0.9256 (2)	1.10816 (18)	0.0572 (5)
H15A	0.8621	0.9817	1.1222	0.069*
C14	1.0666 (2)	0.9379 (2)	1.2097 (2)	0.0681 (5)
H14A	1.1105	1.0055	1.2951	0.082*
C12	1.0973 (2)	0.7530 (2)	1.0670 (2)	0.0700 (6)
H12A	1.1552	0.6963	1.0544	0.084*
C4	−0.0434 (2)	0.7351 (2)	0.4537 (2)	0.0730 (6)
H4B	−0.1279	0.7702	0.4256	0.088*
C13	1.1537 (2)	0.8527 (3)	1.1903 (2)	0.0722 (6)
H13A	1.2527	0.8644	1.2635	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0665 (7)	0.0814 (8)	0.0574 (6)	0.0381 (6)	0.0304 (6)	0.0078 (6)
O2	0.0450 (6)	0.0557 (7)	0.0394 (6)	0.0108 (5)	0.0174 (5)	0.0130 (5)
O1	0.0720 (9)	0.0846 (9)	0.0491 (7)	0.0428 (8)	0.0279 (7)	0.0073 (7)
N1	0.0438 (8)	0.0528 (8)	0.0434 (7)	0.0151 (6)	0.0222 (6)	0.0072 (6)
C6	0.0414 (9)	0.0447 (9)	0.0425 (9)	0.0117 (7)	0.0193 (7)	0.0095 (7)
O3	0.0738 (9)	0.0597 (8)	0.0571 (8)	−0.0010 (7)	0.0295 (7)	0.0072 (7)
C17	0.0388 (8)	0.0551 (10)	0.0441 (9)	0.0198 (8)	0.0184 (7)	0.0178 (8)
C16	0.0409 (9)	0.0503 (10)	0.0478 (9)	0.0157 (8)	0.0200 (8)	0.0154 (8)
C1	0.0448 (9)	0.0510 (10)	0.0501 (10)	0.0157 (8)	0.0242 (8)	0.0109 (8)
N2	0.0558 (10)	0.0667 (10)	0.0553 (9)	0.0160 (8)	0.0290 (8)	−0.0015 (8)
C7	0.0470 (9)	0.0448 (9)	0.0445 (9)	0.0155 (7)	0.0234 (8)	0.0091 (7)
C10	0.0413 (9)	0.0528 (10)	0.0458 (9)	0.0148 (8)	0.0229 (8)	0.0134 (8)
C8	0.0451 (9)	0.0486 (9)	0.0357 (8)	0.0167 (7)	0.0171 (7)	0.0079 (7)
C9	0.0466 (9)	0.0534 (10)	0.0446 (9)	0.0173 (8)	0.0205 (8)	0.0147 (8)
C11	0.0487 (10)	0.0600 (11)	0.0598 (11)	0.0201 (9)	0.0321 (9)	0.0135 (9)
C2	0.0621 (12)	0.0641 (12)	0.0444 (10)	0.0116 (10)	0.0239 (9)	0.0032 (9)
N3	0.0610 (10)	0.0742 (11)	0.0722 (11)	0.0265 (9)	0.0363 (9)	0.0007 (9)
N4	0.0835 (12)	0.0832 (13)	0.0519 (9)	0.0279 (10)	0.0319 (9)	0.0221 (9)
C18	0.0616 (11)	0.0549 (11)	0.0467 (10)	0.0169 (9)	0.0225 (9)	0.0179 (8)
C5	0.0534 (11)	0.0624 (11)	0.0549 (11)	0.0246 (9)	0.0185 (9)	0.0058 (9)
C20	0.0790 (14)	0.0865 (15)	0.0598 (12)	0.0287 (12)	0.0406 (11)	0.0357 (12)
C21	0.0626 (12)	0.0595 (11)	0.0622 (12)	0.0169 (9)	0.0337 (10)	0.0234 (9)
C3	0.0577 (12)	0.0771 (14)	0.0476 (11)	0.0116 (11)	0.0092 (9)	0.0117 (10)
C19	0.0807 (14)	0.0629 (12)	0.0501 (11)	0.0169 (11)	0.0245 (10)	0.0115 (10)
C15	0.0551 (11)	0.0655 (11)	0.0477 (10)	0.0227 (9)	0.0229 (9)	0.0076 (9)

C14	0.0570 (12)	0.0857 (15)	0.0489 (11)	0.0207 (11)	0.0185 (10)	0.0094 (10)
C12	0.0528 (12)	0.0891 (15)	0.0828 (15)	0.0365 (11)	0.0369 (11)	0.0288 (13)
C4	0.0540 (12)	0.0809 (14)	0.0653 (13)	0.0293 (11)	0.0103 (10)	0.0124 (11)
C13	0.0483 (11)	0.1031 (17)	0.0608 (13)	0.0257 (11)	0.0197 (10)	0.0277 (12)

Geometric parameters (Å, °)

F1—C1	1.3583 (19)	C11—C12	1.402 (3)
O2—C16	1.343 (2)	C2—C3	1.373 (3)
O2—C8	1.4378 (19)	C2—H2B	0.9300
O1—C7	1.2116 (19)	N4—C19	1.325 (3)
N1—N2	1.3569 (19)	N4—C20	1.330 (3)
N1—C10	1.362 (2)	C18—C19	1.377 (3)
N1—C9	1.449 (2)	C18—H18A	0.9300
C6—C1	1.384 (2)	C5—C4	1.371 (3)
C6—C5	1.400 (2)	C5—H5A	0.9300
C6—C7	1.491 (2)	C20—C21	1.382 (3)
O3—C16	1.199 (2)	C20—H20A	0.9300
C17—C21	1.379 (2)	C21—H21A	0.9300
C17—C18	1.380 (2)	C3—C4	1.377 (3)
C17—C16	1.488 (2)	C3—H3B	0.9300
C1—C2	1.373 (2)	C19—H19A	0.9300
N2—N3	1.302 (2)	C15—C14	1.362 (3)
C7—C8	1.533 (2)	C15—H15A	0.9300
C10—C11	1.388 (2)	C14—C13	1.400 (3)
C10—C15	1.393 (2)	C14—H14A	0.9300
C8—C9	1.519 (2)	C12—C13	1.364 (3)
C8—H8A	0.9800	C12—H12A	0.9300
C9—H9A	0.9700	C4—H4B	0.9300
C9—H9B	0.9700	C13—H13A	0.9300
C11—N3	1.377 (2)		
C16—O2—C8	116.12 (13)	C1—C2—C3	118.30 (18)
N2—N1—C10	110.20 (14)	C1—C2—H2B	120.9
N2—N1—C9	119.86 (14)	C3—C2—H2B	120.9
C10—N1—C9	129.81 (14)	N2—N3—C11	108.27 (14)
C1—C6—C5	116.08 (15)	C19—N4—C20	116.08 (17)
C1—C6—C7	126.52 (15)	C19—C18—C17	118.69 (17)
C5—C6—C7	117.39 (15)	C19—C18—H18A	120.7
C21—C17—C18	117.94 (16)	C17—C18—H18A	120.7
C21—C17—C16	119.07 (16)	C4—C5—C6	121.40 (18)
C18—C17—C16	122.90 (15)	C4—C5—H5A	119.3
O3—C16—O2	123.54 (16)	C6—C5—H5A	119.3
O3—C16—C17	124.57 (16)	N4—C20—C21	124.06 (18)
O2—C16—C17	111.86 (14)	N4—C20—H20A	118.0
F1—C1—C2	117.06 (15)	C21—C20—H20A	118.0
F1—C1—C6	119.34 (15)	C17—C21—C20	118.72 (19)
C2—C1—C6	123.60 (17)	C17—C21—H21A	120.6
N3—N2—N1	108.73 (14)	C20—C21—H21A	120.6
O1—C7—C6	120.61 (15)	C2—C3—C4	120.54 (18)

O1—C7—C8	118.60 (15)	C2—C3—H3B	119.7
C6—C7—C8	120.73 (14)	C4—C3—H3B	119.7
N1—C10—C11	104.13 (15)	N4—C19—C18	124.45 (19)
N1—C10—C15	133.31 (16)	N4—C19—H19A	117.8
C11—C10—C15	122.52 (16)	C18—C19—H19A	117.8
O2—C8—C9	105.69 (13)	C14—C15—C10	115.87 (17)
O2—C8—C7	108.33 (12)	C14—C15—H15A	122.1
C9—C8—C7	111.49 (13)	C10—C15—H15A	122.1
O2—C8—H8A	110.4	C15—C14—C13	122.52 (19)
C9—C8—H8A	110.4	C15—C14—H14A	118.7
C7—C8—H8A	110.4	C13—C14—H14A	118.7
N1—C9—C8	111.36 (13)	C13—C12—C11	116.90 (18)
N1—C9—H9A	109.4	C13—C12—H12A	121.6
C8—C9—H9A	109.4	C11—C12—H12A	121.6
N1—C9—H9B	109.4	C5—C4—C3	120.06 (19)
C8—C9—H9B	109.4	C5—C4—H4B	120.0
H9A—C9—H9B	108.0	C3—C4—H4B	120.0
N3—C11—C10	108.67 (16)	C12—C13—C14	121.70 (19)
N3—C11—C12	130.83 (17)	C12—C13—H13A	119.2
C10—C11—C12	120.49 (18)	C14—C13—H13A	119.2
C8—O2—C16—O3	9.6 (2)	N1—C10—C11—N3	0.32 (19)
C8—O2—C16—C17	−168.46 (12)	C15—C10—C11—N3	−177.61 (16)
C21—C17—C16—O3	15.3 (3)	N1—C10—C11—C12	179.33 (16)
C18—C17—C16—O3	−161.11 (18)	C15—C10—C11—C12	1.4 (3)
C21—C17—C16—O2	−166.66 (14)	F1—C1—C2—C3	178.98 (16)
C18—C17—C16—O2	16.9 (2)	C6—C1—C2—C3	−0.1 (3)
C5—C6—C1—F1	−177.74 (15)	N1—N2—N3—C11	0.2 (2)
C7—C6—C1—F1	1.1 (3)	C10—C11—N3—N2	−0.3 (2)
C5—C6—C1—C2	1.3 (3)	C12—C11—N3—N2	−179.20 (19)
C7—C6—C1—C2	−179.83 (17)	C21—C17—C18—C19	−2.0 (3)
C10—N1—N2—N3	0.0 (2)	C16—C17—C18—C19	174.45 (17)
C9—N1—N2—N3	−176.20 (14)	C1—C6—C5—C4	−1.6 (3)
C1—C6—C7—O1	−174.06 (17)	C7—C6—C5—C4	179.40 (18)
C5—C6—C7—O1	4.8 (2)	C19—N4—C20—C21	−2.2 (3)
C1—C6—C7—C8	8.8 (3)	C18—C17—C21—C20	0.1 (3)
C5—C6—C7—C8	−172.32 (15)	C16—C17—C21—C20	−176.54 (17)
N2—N1—C10—C11	−0.20 (18)	N4—C20—C21—C17	2.2 (3)
C9—N1—C10—C11	175.51 (15)	C1—C2—C3—C4	−0.9 (3)
N2—N1—C10—C15	177.39 (18)	C20—N4—C19—C18	0.0 (3)
C9—N1—C10—C15	−6.9 (3)	C17—C18—C19—N4	2.1 (3)
C16—O2—C8—C9	−166.09 (13)	N1—C10—C15—C14	−177.50 (18)
C16—O2—C8—C7	74.31 (17)	C11—C10—C15—C14	−0.3 (3)
O1—C7—C8—O2	13.9 (2)	C10—C15—C14—C13	−0.9 (3)
C6—C7—C8—O2	−168.92 (13)	N3—C11—C12—C13	177.4 (2)
O1—C7—C8—C9	−101.99 (18)	C10—C11—C12—C13	−1.3 (3)
C6—C7—C8—C9	75.19 (19)	C6—C5—C4—C3	0.7 (3)
N2—N1—C9—C8	86.68 (18)	C2—C3—C4—C5	0.6 (3)
C10—N1—C9—C8	−88.7 (2)	C11—C12—C13—C14	0.2 (3)
O2—C8—C9—N1	69.41 (16)	C15—C14—C13—C12	1.0 (3)

C7—C8—C9—N1	−173.09 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2B···N3^{i}	0.93	2.50	3.427 (3)	172
C8—H8A···F1	0.98	2.25	2.759 (2)	112
C15—H15A···O1^{ii}	0.93	2.54	3.452 (3)	168
C21—H21A···N2^{iii}	0.93	2.57	3.398 (3)	148

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

Fig. 1

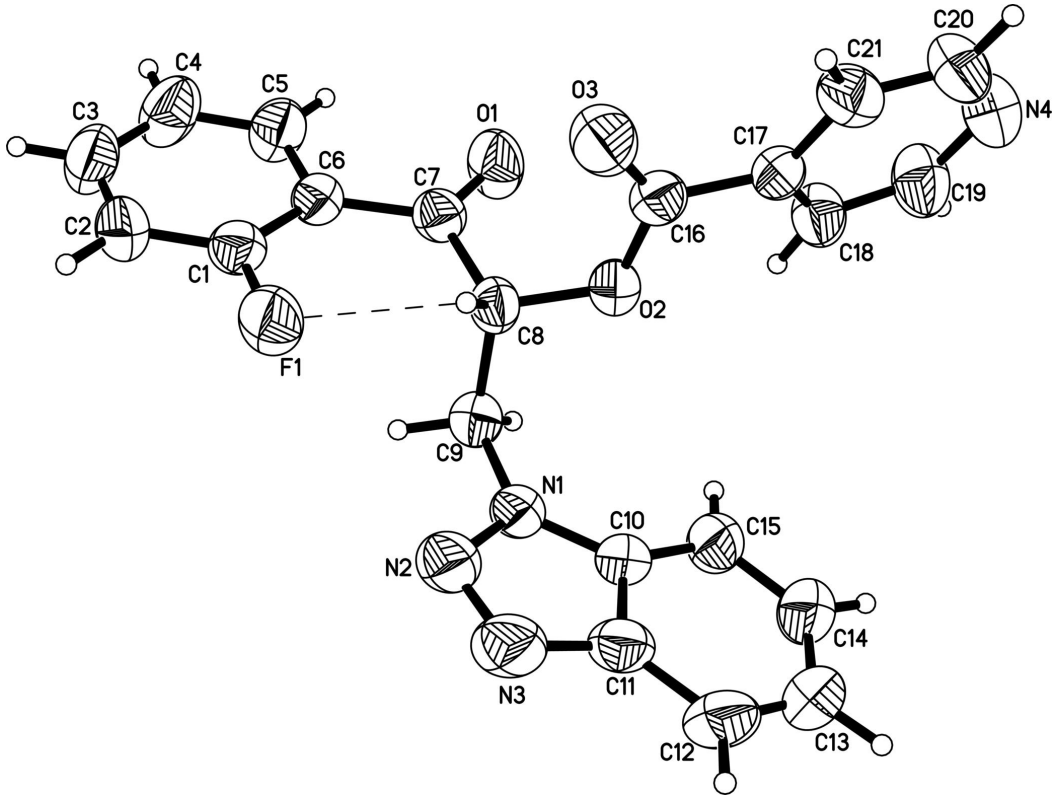
C20
C21
C4
C5
O3
N4
C3
O1
C17
C6
C7
C19
C2
C16
C18
C1
O2
F1
C8
C9
N1
C10
C15
N2
C14
N3
C11
C12
C13

Fig. 2