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3-(1*H*-Benzotriazol-1-yl)-1-(2-fluorobenzoyl)ethyl nicotinate

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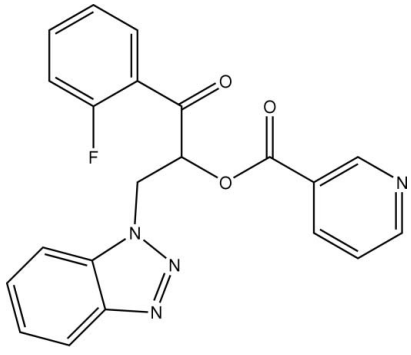
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.114; data-to-parameter ratio = 13.5.

In the molecule of the title compound, $C_{21}H_{15}FN_4O_3$, intramolecular C—H···O and C—H···F hydrogen bonds result in the formation of one six- and one five-membered ring. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules into chains along the *a* axis. The packing is further stabilized by π–π interactions [centroid–centroid distance 3.632 (2) Å].

Related literature

For related literature, see: Han *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{15}FN_4O_3$
M_r = 390.37
Triclinic, $P\overline{1}$
a = 9.8423 (9) Å
b = 9.9736 (10) Å
c = 11.4000 (11) Å
α = 64.459 (1)°
β = 67.157 (1)°
γ = 76.313 (1)°
V = 927.28 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.36 × 0.30 × 0.26 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.974
5202 measured reflections
3560 independent reflections
2877 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.114
S = 1.05
3560 reflections
263 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
C3—H3*B*···O3^{i}	0.93	2.50	3.355 (2)	154
C8—H8*A*···F1	0.98	2.23	2.747 (2)	112
C9—H9*B*···O1^{ii}	0.97	2.53	3.464 (2)	161
C18—H18*A*···O2	0.93	2.43	2.758 (2)	101

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

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: HK2319).

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supplementary materials

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3-(1*H*-Benzotriazol-1-yl)-1-(2-fluorobenzoyl)ethyl nicotinate

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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 crystal structure is reported here.

In the molecule of the title compound, (I), the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987), and are comparable to those in the related compound (II). In (I), the benzotriazole ring system is essentially planar with a dihedral angle of 0.45 (1)° between triazole A (N1—N3/C10/C11) and benzene B (C10—C15) rings. Rings C (N4/C17—C21) and D (C1—C6) are oriented with respect to the benzotriazole system at dihedral angles of 87.82 (1)° and 0.78 (1)°, respectively, while the dihedral angle between them is 87.62 (1)°. The intramolecular C—H···O and C—H···F hydrogen bonds (Table 1) cause to the formation of one six- and one five-membered rings (Fig. 1).

In the crystal structure, the intermolecular C—H···O hydrogen bonds (Table 1), link the molecules into chains along the *a* axis (Fig. 2). The packing is further stabilized by π-π interactions involving the C1—C6 benzene rings: $Cg3\cdots Cg3^{iv}$ = 3.632 Å [symmetry code: (iv) 2 − *x*, −*y*, −1 − *z*, *Cg*3 is the centroid of th benzene ring].

Experimental

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

Refinement

H atoms were positioned geometrically with C—H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C)

Figures

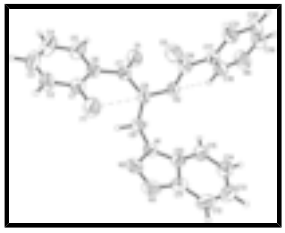

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

3-(1*H*-Benzotriazol-1-yl)-1-(2-fluorobenzoyl)ethyl nicotinate

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
$a = 9.8423$ (9) Å	Cell parameters from 2193 reflections
$b = 9.9736$ (10) Å	$\theta = 2.3$–24.9°
$c = 11.4000$ (11) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 64.459$ (1)°	$T = 298$ (2) K
$\beta = 67.157$ (1)°	Block, yellow
$\gamma = 76.313$ (1)°	0.36 × 0.30 × 0.26 mm
$V = 927.28$ (15) Å^3	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3560 independent reflections
Radiation source: fine-focus sealed tube	2877 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.013$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.0^\circ$
$T = 293$(2) K	$\theta_{min} = 2.1^\circ$
ω scans	$h = -12 \rightarrow 6$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -12 \rightarrow 12$
$T_{min} = 0.964$, $T_{max} = 0.974$	$l = -14 \rightarrow 14$
5202 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.1733P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.114$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.14$ e Å^{-3}
3560 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}
263 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.026 (3)
Secondary atom site location: difference Fourier map	

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	0.89959 (13)	0.26256 (12)	−0.41995 (10)	0.0754 (4)
O1	0.65340 (14)	−0.09185 (13)	−0.12652 (11)	0.0621 (3)
O2	0.72673 (11)	0.03294 (11)	−0.00182 (9)	0.0444 (3)
O3	0.94370 (14)	−0.10059 (14)	−0.05293 (12)	0.0660 (4)
N1	0.68866 (14)	0.36422 (13)	−0.13452 (12)	0.0433 (3)
N2	0.77269 (15)	0.47243 (14)	−0.24241 (14)	0.0539 (4)
N3	0.80732 (16)	0.55330 (15)	−0.19591 (15)	0.0592 (4)
N4	0.59613 (19)	−0.25912 (19)	0.39906 (15)	0.0761 (5)
C1	0.85535 (18)	0.17262 (17)	−0.45709 (16)	0.0487 (4)
C2	0.9011 (2)	0.2013 (2)	−0.59553 (17)	0.0607 (5)
H2B	0.9598	0.2790	−0.6596	0.073*
C3	0.8578 (2)	0.1122 (2)	−0.63630 (19)	0.0696 (5)
H3B	0.8860	0.1305	−0.7294	0.084*
C4	0.7734 (2)	−0.0035 (3)	−0.5410 (2)	0.0749 (6)
H4B	0.7447	−0.0634	−0.5697	0.090*
C5	0.73070 (19)	−0.0316 (2)	−0.40328 (18)	0.0592 (5)
H5A	0.6746	−0.1115	−0.3398	0.071*
C6	0.76984 (16)	0.05731 (16)	−0.35668 (15)	0.0420 (3)
C7	0.72116 (16)	0.01687 (16)	−0.20536 (15)	0.0416 (3)
C8	0.75139 (16)	0.11471 (15)	−0.14647 (14)	0.0406 (3)
H8A	0.8533	0.1432	−0.1937	0.049*
C9	0.64266 (17)	0.25315 (16)	−0.15857 (15)	0.0430 (3)
H9A	0.6338	0.2963	−0.2498	0.052*
H9B	0.5460	0.2246	−0.0924	0.052*
C10	0.66910 (16)	0.37656 (15)	−0.01425 (15)	0.0424 (3)
C11	0.74604 (18)	0.49795 (17)	−0.05488 (18)	0.0501 (4)
C12	0.7507 (2)	0.5446 (2)	0.0431 (2)	0.0672 (5)
H12A	0.8022	0.6253	0.0175	0.081*
C13	0.6769 (2)	0.4668 (2)	0.1771 (2)	0.0705 (5)
H13A	0.6782	0.4951	0.2444	0.085*
C14	0.5989 (2)	0.3452 (2)	0.21693 (19)	0.0648 (5)
H14A	0.5497	0.2954	0.3098	0.078*
C15	0.59284 (19)	0.29725 (18)	0.12321 (16)	0.0532 (4)

H15A	0.5409	0.2166	0.1497	0.064*
C16	0.82944 (17)	−0.07994 (16)	0.03048 (15)	0.0424 (3)
C17	0.78394 (16)	−0.17652 (15)	0.17859 (15)	0.0413 (3)
C18	0.64180 (19)	−0.16715 (19)	0.26721 (16)	0.0554 (4)
H18A	0.5741	−0.0926	0.2332	0.066*
C19	0.6977 (3)	−0.3626 (2)	0.44441 (19)	0.0743 (6)
H19A	0.6687	−0.4275	0.5360	0.089*
C20	0.8409 (2)	−0.37952 (19)	0.36566 (19)	0.0638 (5)
H20A	0.9073	−0.4527	0.4033	0.077*
C21	0.88514 (19)	−0.28663 (17)	0.22992 (17)	0.0528 (4)
H21A	0.9815	−0.2972	0.1731	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1104 (9)	0.0647 (7)	0.0472 (6)	−0.0452 (6)	−0.0100 (6)	−0.0125 (5)
O1	0.0804 (8)	0.0543 (7)	0.0468 (7)	−0.0304 (6)	−0.0125 (6)	−0.0097 (5)
O2	0.0525 (6)	0.0432 (6)	0.0325 (5)	0.0024 (5)	−0.0155 (5)	−0.0117 (4)
O3	0.0592 (7)	0.0693 (8)	0.0489 (7)	0.0123 (6)	−0.0107 (6)	−0.0192 (6)
N1	0.0509 (7)	0.0341 (6)	0.0392 (7)	−0.0053 (5)	−0.0133 (6)	−0.0090 (5)
N2	0.0618 (8)	0.0377 (7)	0.0470 (8)	−0.0077 (6)	−0.0109 (6)	−0.0067 (6)
N3	0.0655 (9)	0.0405 (7)	0.0637 (9)	−0.0134 (6)	−0.0132 (7)	−0.0150 (7)
N4	0.0797 (11)	0.0737 (11)	0.0437 (8)	0.0012 (9)	−0.0101 (8)	−0.0072 (8)
C1	0.0556 (9)	0.0452 (8)	0.0424 (8)	−0.0058 (7)	−0.0139 (7)	−0.0152 (7)
C2	0.0640 (11)	0.0623 (11)	0.0390 (9)	−0.0032 (9)	−0.0076 (8)	−0.0133 (8)
C3	0.0701 (12)	0.0952 (15)	0.0451 (10)	0.0061 (11)	−0.0163 (9)	−0.0368 (10)
C4	0.0765 (13)	0.1037 (16)	0.0658 (12)	−0.0143 (12)	−0.0180 (10)	−0.0523 (12)
C5	0.0573 (10)	0.0714 (11)	0.0567 (10)	−0.0162 (9)	−0.0099 (8)	−0.0334 (9)
C6	0.0418 (8)	0.0440 (8)	0.0396 (8)	−0.0017 (6)	−0.0125 (6)	−0.0169 (6)
C7	0.0432 (8)	0.0391 (7)	0.0398 (8)	−0.0059 (6)	−0.0135 (6)	−0.0112 (6)
C8	0.0461 (8)	0.0405 (8)	0.0317 (7)	−0.0070 (6)	−0.0117 (6)	−0.0098 (6)
C9	0.0489 (8)	0.0402 (8)	0.0398 (8)	−0.0040 (6)	−0.0180 (7)	−0.0116 (6)
C10	0.0435 (8)	0.0372 (7)	0.0462 (8)	0.0025 (6)	−0.0169 (7)	−0.0166 (6)
C11	0.0509 (9)	0.0380 (8)	0.0607 (10)	−0.0013 (7)	−0.0186 (8)	−0.0189 (7)
C12	0.0780 (13)	0.0521 (10)	0.0888 (15)	−0.0037 (9)	−0.0355 (11)	−0.0356 (10)
C13	0.0881 (14)	0.0685 (12)	0.0761 (14)	0.0069 (11)	−0.0382 (11)	−0.0431 (11)
C14	0.0776 (13)	0.0669 (11)	0.0501 (10)	0.0029 (10)	−0.0199 (9)	−0.0275 (9)
C15	0.0581 (10)	0.0512 (9)	0.0469 (9)	−0.0086 (8)	−0.0127 (8)	−0.0176 (7)
C16	0.0473 (8)	0.0415 (8)	0.0420 (8)	0.0001 (6)	−0.0176 (7)	−0.0185 (7)
C17	0.0503 (8)	0.0387 (7)	0.0411 (8)	−0.0015 (6)	−0.0210 (7)	−0.0163 (6)
C18	0.0585 (10)	0.0539 (9)	0.0438 (9)	0.0045 (8)	−0.0190 (8)	−0.0124 (7)
C19	0.1031 (17)	0.0611 (11)	0.0426 (10)	−0.0030 (11)	−0.0272 (11)	−0.0043 (8)
C20	0.0812 (13)	0.0489 (10)	0.0616 (11)	0.0050 (9)	−0.0412 (10)	−0.0109 (8)
C21	0.0559 (10)	0.0469 (9)	0.0571 (10)	0.0020 (7)	−0.0272 (8)	−0.0165 (8)

Geometric parameters (Å, °)

F1—C1	1.3525 (19)	C8—H8A	0.9800
O1—C7	1.2103 (17)	C9—H9A	0.9700

O2—C8	1.4376 (16)	C9—H9B	0.9700
O2—C16	1.3482 (17)	C10—C11	1.390 (2)
O3—C16	1.2001 (18)	C10—C15	1.394 (2)
N1—N2	1.3600 (17)	C11—C12	1.401 (3)
N1—C9	1.4501 (19)	C12—H12A	0.9300
N1—C10	1.3643 (19)	C13—C12	1.359 (3)
N3—N2	1.299 (2)	C13—H13A	0.9300
N3—C11	1.376 (2)	C14—C15	1.370 (2)
N4—C19	1.336 (2)	C14—C13	1.401 (3)
C1—C2	1.377 (2)	C14—H14A	0.9300
C2—C3	1.369 (3)	C15—H15A	0.9300
C2—H2B	0.9300	C16—C17	1.481 (2)
C3—C4	1.369 (3)	C17—C18	1.382 (2)
C3—H3B	0.9300	C17—C21	1.386 (2)
C4—H4B	0.9300	C18—N4	1.336 (2)
C5—C4	1.372 (3)	C18—H18A	0.9300
C5—H5A	0.9300	C19—H19A	0.9300
C6—C1	1.384 (2)	C20—C19	1.363 (3)
C6—C5	1.394 (2)	C20—H20A	0.9300
C7—C6	1.489 (2)	C21—C20	1.369 (2)
C7—C8	1.533 (2)	C21—H21A	0.9300
C8—C9	1.524 (2)		
C16—O2—C8	115.43 (11)	C8—C9—H9B	109.2
N2—N1—C10	109.94 (12)	H9A—C9—H9B	107.9
N2—N1—C9	119.71 (12)	N1—C10—C11	104.16 (13)
C10—N1—C9	130.22 (12)	N1—C10—C15	133.48 (14)
N3—N2—N1	108.89 (13)	C11—C10—C15	122.35 (15)
N2—N3—C11	108.38 (13)	N3—C11—C10	108.63 (14)
C18—N4—C19	116.17 (17)	N3—C11—C12	130.90 (16)
F1—C1—C2	116.89 (15)	C10—C11—C12	120.47 (16)
F1—C1—C6	119.52 (13)	C13—C12—C11	117.14 (17)
C2—C1—C6	123.58 (16)	C13—C12—H12A	121.4
C3—C2—C1	118.23 (17)	C11—C12—H12A	121.4
C3—C2—H2B	120.9	C12—C13—C14	121.96 (18)
C1—C2—H2B	120.9	C12—C13—H13A	119.0
C2—C3—C4	120.45 (17)	C14—C13—H13A	119.0
C2—C3—H3B	119.8	C15—C14—C13	122.02 (18)
C4—C3—H3B	119.8	C15—C14—H14A	119.0
C3—C4—C5	120.44 (18)	C13—C14—H14A	119.0
C3—C4—H4B	119.8	C14—C15—C10	116.06 (16)
C5—C4—H4B	119.8	C14—C15—H15A	122.0
C4—C5—C6	121.31 (17)	C10—C15—H15A	122.0
C4—C5—H5A	119.3	O3—C16—O2	123.21 (14)
C6—C5—H5A	119.3	O3—C16—C17	124.15 (14)
C1—C6—C5	115.97 (14)	O2—C16—C17	112.63 (12)
C1—C6—C7	126.34 (14)	C18—C17—C21	118.07 (14)
C5—C6—C7	117.65 (14)	C18—C17—C16	122.75 (13)
O1—C7—C6	120.59 (13)	C21—C17—C16	119.08 (14)
O1—C7—C8	118.64 (13)	N4—C18—C17	123.69 (15)

C6—C7—C8	120.73 (12)	N4—C18—H18A	118.2
O2—C8—C9	106.13 (11)	C17—C18—H18A	118.2
O2—C8—C7	108.81 (11)	N4—C19—C20	124.51 (17)
C9—C8—C7	110.90 (12)	N4—C19—H19A	117.7
O2—C8—H8A	110.3	C20—C19—H19A	117.7
C9—C8—H8A	110.3	C19—C20—C21	118.61 (16)
C7—C8—H8A	110.3	C19—C20—H20A	120.7
N1—C9—C8	112.17 (12)	C21—C20—H20A	120.7
N1—C9—H9A	109.2	C20—C21—C17	118.91 (16)
C8—C9—H9A	109.2	C20—C21—H21A	120.5
N1—C9—H9B	109.2	C17—C21—H21A	120.5
C16—O2—C8—C9	−168.65 (11)	C8—C7—C6—C5	−176.13 (14)
C16—O2—C8—C7	71.94 (15)	O1—C7—C8—O2	15.96 (19)
C8—O2—C16—O3	9.4 (2)	C6—C7—C8—O2	−165.99 (12)
C8—O2—C16—C17	−169.32 (11)	O1—C7—C8—C9	−100.42 (16)
C10—N1—N2—N3	−0.08 (17)	C6—C7—C8—C9	77.63 (16)
C9—N1—N2—N3	−176.40 (12)	O2—C8—C9—N1	75.59 (14)
N2—N1—C9—C8	91.87 (15)	C7—C8—C9—N1	−166.39 (11)
C10—N1—C9—C8	−83.59 (18)	N1—C10—C11—N3	0.26 (16)
N2—N1—C10—C11	−0.11 (15)	C15—C10—C11—N3	−179.16 (14)
C9—N1—C10—C11	175.70 (14)	N1—C10—C11—C12	−179.94 (14)
N2—N1—C10—C15	179.21 (16)	C15—C10—C11—C12	0.6 (2)
C9—N1—C10—C15	−5.0 (3)	N1—C10—C15—C14	−179.72 (16)
C11—N3—N2—N1	0.24 (17)	C11—C10—C15—C14	−0.5 (2)
N2—N3—C11—C10	−0.32 (18)	N3—C11—C12—C13	179.43 (17)
N2—N3—C11—C12	179.91 (17)	C10—C11—C12—C13	−0.3 (3)
C18—N4—C19—C20	−0.4 (3)	C14—C13—C12—C11	−0.1 (3)
F1—C1—C2—C3	−179.88 (15)	C13—C14—C15—C10	0.1 (3)
C6—C1—C2—C3	1.0 (3)	C15—C14—C13—C12	0.2 (3)
C1—C2—C3—C4	−1.1 (3)	C18—C17—C21—C20	−0.8 (2)
C2—C3—C4—C5	0.1 (3)	C16—C17—C21—C20	−177.42 (15)
C6—C5—C4—C3	0.9 (3)	C21—C17—C18—N4	−0.7 (3)
C5—C6—C1—F1	−179.08 (14)	C16—C17—C18—N4	175.74 (16)
C7—C6—C1—F1	−1.4 (2)	O3—C16—C17—C18	−167.62 (16)
C5—C6—C1—C2	0.0 (2)	O2—C16—C17—C18	11.0 (2)
C7—C6—C1—C2	177.67 (15)	O3—C16—C17—C21	8.8 (2)
C1—C6—C5—C4	−1.0 (3)	O2—C16—C17—C21	−172.55 (13)
C7—C6—C5—C4	−178.86 (17)	C17—C18—N4—C19	1.3 (3)
O1—C7—C6—C1	−175.75 (15)	C21—C20—C19—N4	−1.1 (3)
C8—C7—C6—C1	6.2 (2)	C17—C21—C20—C19	1.7 (3)
O1—C7—C6—C5	1.9 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3B···O3^{i}	0.93	2.50	3.355 (2)	154
C8—H8A···F1	0.98	2.23	2.747 (2)	112
C9—H9B···O1^{ii}	0.97	2.53	3.464 (2)	161

C18—H18A···O2	0.93	2.43	2.758 (2)	101

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

Fig. 1

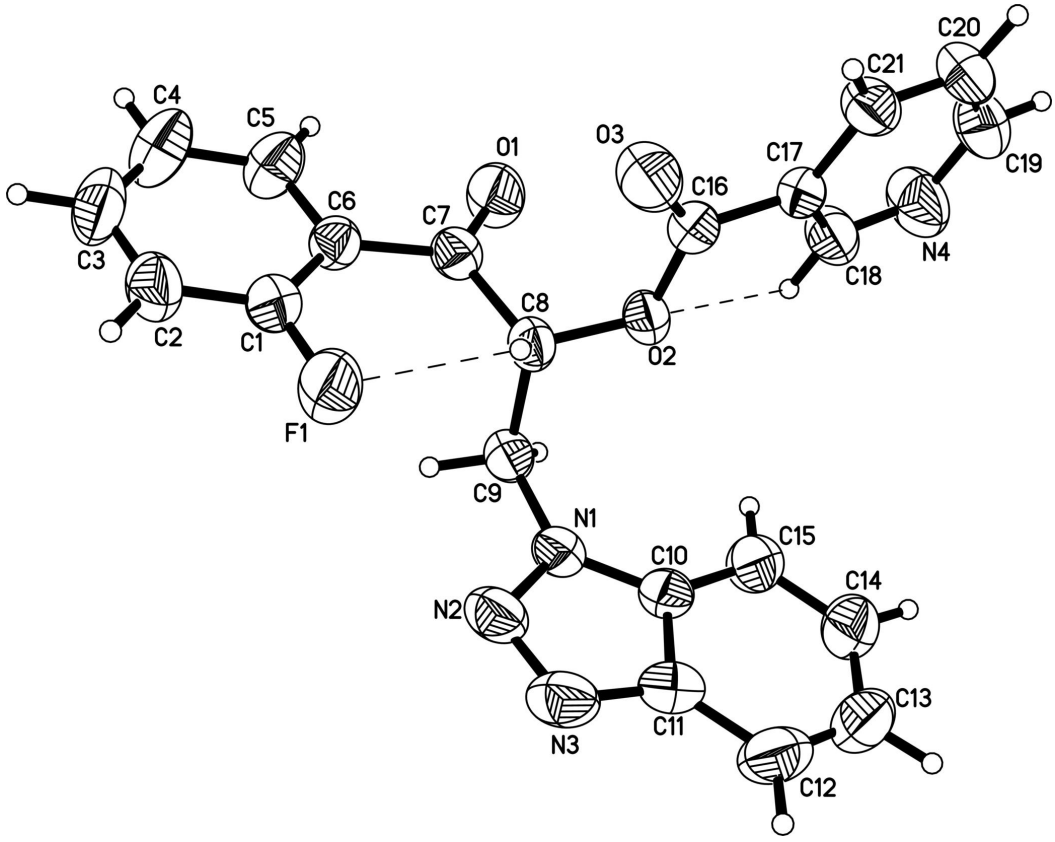

Fig. 2