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# Ethyl 1-*sec*-butyl-2-(4-fluorophenyl)-1*H*-benzimidazole-5-carboxylate

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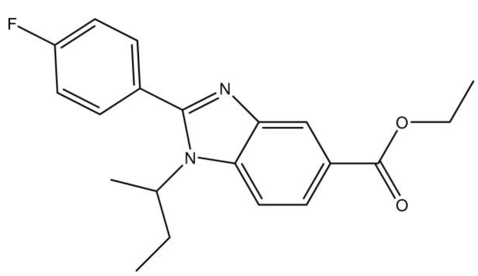
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.047; $wR$ factor = 0.150; data-to-parameter ratio = 13.7.

In the title compound, $C_{20}H_{21}FN_2O_2$, the benzene ring and the benzimidazole ring system are inclined at a dihedral angle of 44.40 (9)°. In the crystal, molecules are linked by intermolecular C—H···O hydrogen bonds, forming a zigzag chain along the $b$-axis direction. An intramolecular C—H···$\pi$ interaction is also observed.

## Related literature

For the synthesis of the title compound and related structures, see: Arumugam, Abd Hamid *et al.* (2010); Arumugam, Abdul Rahim, Osman, Hemamalini & Fun (2010); Arumugam, Abdul Rahim, Osman, Quah & Fun (2010). For applications of benzimidazole derivatives, see: Spasov *et al.* (1999); Easmon *et al.* (2001); Özden *et al.* (2004). For bond-length data, see: Allen *et al.* (1987).




## Experimental

*Crystal data*

$C_{20}H_{21}FN_2O_2$
$M_r$ = 340.39
Monoclinic, $P2_1/c$
$a$ = 10.2249 (16) Å
$b$ = 12.3767 (18) Å
$c$ = 14.149 (2) Å
$\beta$ = 93.473 (2)°
$V$ = 1787.3 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
0.37 × 0.20 × 0.11 mm

*Data collection*

Bruker APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.968, $T_{max}$ = 0.990
10465 measured reflections
3130 independent reflections
2342 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.150
$S$ = 1.05
3130 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

*Cg*1 is the centroid of the N1/C7/N2/C1/C6 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C5—H5···O1$^{i}$ | 0.93 | 2.53 | 3.452 (3) | 169 |
| C20—H20*C*···O1$^{i}$ | 0.96 | 2.59 | 3.485 (4) | 154 |
| C19—H19*A*···*Cg*1 | 0.96 | 2.82 | 3.400 (3) | 121 |

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2787).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o2938 [ **doi:10.1107/S1600536811041663** ]

**Ethyl 1-*sec*-butyl-2-(4-fluorophenyl)-1*H*-benzimidazole-5-carboxylate**

**N. Arumugam, N. Ngah, S. Abd Hamid and A. S. Abdul Rahim**

### Comment

The synthesis of benzimidazole heterocycles is ever fascinating since they promise a wide spectrum of pharmacological activities such as antibacterial (Özden *et al.*, 2004), anticancer (Easmon *et al.*, 2001) and antifungal (Spasov *et al.*, 1999). As the benzimidazole derivative is of much importance, we have undertaken the X-ray crystal structure determination of the title compound.

The title compound (Fig. 1) is similar to those previously reported ethyl-1-*sec*-butyl-2-(4-chlorophenyl)-1*H*-benzimidazole-5-carboxylate (Arumugam, Abdul Rahim, Osman, Quah & Fun, 2010) except the fluorine atom is attached at the *para* position of the phenyl ring. The phenyl (C8/C9/C10/ C11/C12/C13) and benzimidazole (N1/N2/C1/C2/C3/C4/C5) fragments are essentially planar with maximum deviation is 0.005 (2)Å for atom C2. Both fragments are inclined to each other by 44.40 (9)°. The bond lengths are in normal ranges (Allen *et al.*, 1987) and in agreement to those reported by Arumugam *et al.* (Arumugam, Abd Hamid *et al.*, 2010; Arumugam, Abdul Rahim, Osman, Hemamalini & Fun, 2010; Arumugam, Abdul Rahim, Osman, Quah & Fun, 2010). In the crystal structure (Fig. 2), the molecules are linked by intermolecular C5—H5···O1$^{i}$ and C20—H20C···O1$^{i}$ hydrogen bonds (symmetry codes as in Table 1) to form a zigzag chain along the *b* axis. The molecular structure is further stabilized by an intramolecular C—H···*Cg*1 (Table 1) interaction; *Cg*1 is the centroid of the N1/C7/N2/C1/C6 ring.

### Experimental

A solution of ethyl-3-amino-4-(*sec*-butylamino) benzoate (1.0 mmol) and sodium bisulfite adduct of 4-fluorobenzaldehyde (3.5 mmol) in DMF was treated under microwave conditions at 130 °C for 2 minutes. The reaction mixture was diluted in EtOAc (20 ml) and washed with $H_2O$ (20 ml). The organic layer was collected and dried with $Na_2SO_4$. The solvent was evaporated in *vacuo* to afford a crude product. Recrystallization of the crude product gave the title compound as colourless crystal.

### Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.98 Å, and with $U_{iso}$(H)= 1.2 or 1.5$U_{eq}$(C). The rotating group model was applied for methyl groups.

### Figures

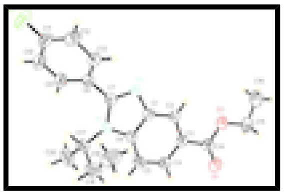

Fig. 1. The molecular structure of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids for non-H atoms.

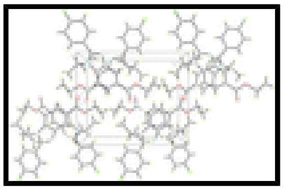

Fig. 2. A molecular packing diagram of the title compound, viewed down the *c* axis.

### Ethyl 1-*sec*-butyl-2-(4-fluorophenyl)-1*H*-benzimidazole- 5-carboxylate

*Crystal data*

| | |
|---|---|
| $C_{20}H_{21}FN_2O_2$ | $F(000) = 720$ |
| $M_r = 340.39$ | $D_x = 1.265$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 2853 reflections |
| $a = 10.2249$ (16) Å | $\theta = 2.0$–25.0° |
| $b = 12.3767$ (18) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 14.149$ (2) Å | $T = 293$ K |
| $\beta = 93.473$ (2)° | Block, colourless |
| $V = 1787.3$ (5) Å$^3$ | 0.37 × 0.20 × 0.11 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII DUO CCD diffractometer | 3130 independent reflections |
| Radiation source: fine-focus sealed tube | 2342 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.027$ |
| Detector resolution: 83.66 pixels mm$^{-1}$ | $\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$ |
| φ and ω scans | $h = -12 \rightarrow 12$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $k = -14 \rightarrow 14$ |
| $T_{min} = 0.968$, $T_{max} = 0.990$ | $l = -16 \rightarrow 16$ |
| 10465 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.047$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.150$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0825P)^2 + 0.313P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3130 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 229 parameters | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.20$ e Å$^{-3}$ |

*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 $F^2 > \sigma(F^2)$ 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 | 1.45030 (16) | 1.11874 (14) | 0.07109 (13) | 0.1053 (6) |
| O1 | 0.49279 (17) | 0.52863 (13) | 0.17567 (13) | 0.0764 (5) |
| O2 | 0.65827 (16) | 0.47066 (12) | 0.09413 (12) | 0.0696 (5) |
| N1 | 0.89771 (15) | 0.92002 (12) | 0.18887 (11) | 0.0456 (4) |
| N2 | 0.98670 (15) | 0.78337 (12) | 0.10912 (11) | 0.0468 (4) |
| C1 | 0.86373 (18) | 0.75303 (14) | 0.13674 (12) | 0.0421 (4) |
| C2 | 0.79676 (19) | 0.65643 (15) | 0.12078 (13) | 0.0458 (5) |
| H2 | 0.8334 | 0.6006 | 0.0872 | 0.055* |
| C3 | 0.67392 (19) | 0.64541 (15) | 0.15618 (13) | 0.0467 (5) |
| C4 | 0.6195 (2) | 0.73015 (17) | 0.20597 (15) | 0.0537 (5) |
| H4 | 0.5372 | 0.7208 | 0.2293 | 0.064* |
| C5 | 0.68326 (19) | 0.82662 (17) | 0.22166 (15) | 0.0542 (5) |
| H5 | 0.6456 | 0.8827 | 0.2543 | 0.065* |
| C6 | 0.80724 (18) | 0.83677 (15) | 0.18631 (13) | 0.0439 (5) |
| C7 | 1.00272 (18) | 0.88255 (15) | 0.14109 (12) | 0.0428 (4) |
| C8 | 1.11991 (18) | 0.94762 (15) | 0.12502 (13) | 0.0443 (5) |
| C9 | 1.1114 (2) | 1.05455 (17) | 0.09460 (14) | 0.0557 (5) |
| H9 | 1.0297 | 1.0875 | 0.0865 | 0.067* |
| C10 | 1.2223 (3) | 1.11195 (19) | 0.07637 (16) | 0.0658 (6) |
| H10 | 1.2166 | 1.1834 | 0.0561 | 0.079* |
| C11 | 1.3408 (2) | 1.0617 (2) | 0.08865 (17) | 0.0672 (6) |
| C12 | 1.3540 (2) | 0.9576 (2) | 0.11717 (18) | 0.0697 (7) |
| H12 | 1.4361 | 0.9253 | 0.1240 | 0.084* |
| C13 | 1.2422 (2) | 0.90061 (18) | 0.13581 (16) | 0.0582 (6) |

| | | | | |
|---|---|---|---|---|
| H13 | 1.2496 | 0.8293 | 0.1560 | 0.070* |
| C14 | 0.5983 (2) | 0.54440 (17) | 0.14437 (14) | 0.0528 (5) |
| C15 | 0.5918 (3) | 0.36793 (19) | 0.0794 (2) | 0.0798 (8) |
| H15A | 0.5018 | 0.3795 | 0.0559 | 0.096* |
| H15B | 0.5915 | 0.3282 | 0.1385 | 0.096* |
| C16 | 0.6626 (3) | 0.3076 (2) | 0.0104 (2) | 0.0967 (10) |
| H16A | 0.6615 | 0.3474 | −0.0479 | 0.145* |
| H16B | 0.6213 | 0.2387 | −0.0007 | 0.145* |
| H16C | 0.7515 | 0.2970 | 0.0342 | 0.145* |
| C17 | 0.8973 (2) | 1.01576 (17) | 0.25156 (16) | 0.0608 (6) |
| H17 | 0.9825 | 1.0513 | 0.2477 | 0.073* |
| C18 | 0.8868 (3) | 0.9822 (2) | 0.35314 (18) | 0.0803 (8) |
| H18A | 0.8993 | 1.0451 | 0.3935 | 0.096* |
| H18B | 0.7994 | 0.9545 | 0.3610 | 0.096* |
| C19 | 0.9833 (3) | 0.8994 (3) | 0.38342 (18) | 0.0906 (9) |
| H19A | 0.9644 | 0.8337 | 0.3492 | 0.136* |
| H19B | 0.9789 | 0.8864 | 0.4500 | 0.136* |
| H19C | 1.0696 | 0.9240 | 0.3708 | 0.136* |
| C20 | 0.7917 (3) | 1.0977 (2) | 0.2147 (3) | 0.0974 (10) |
| H20A | 0.7997 | 1.1099 | 0.1483 | 0.146* |
| H20B | 0.8036 | 1.1647 | 0.2483 | 0.146* |
| H20C | 0.7062 | 1.0693 | 0.2246 | 0.146* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0832 (11) | 0.1053 (12) | 0.1309 (14) | −0.0492 (9) | 0.0352 (10) | 0.0009 (10) |
| O1 | 0.0610 (10) | 0.0656 (11) | 0.1054 (13) | −0.0198 (8) | 0.0281 (9) | −0.0043 (9) |
| O2 | 0.0676 (10) | 0.0470 (9) | 0.0966 (11) | −0.0210 (7) | 0.0245 (9) | −0.0150 (8) |
| N1 | 0.0434 (9) | 0.0390 (9) | 0.0552 (9) | −0.0022 (7) | 0.0100 (7) | −0.0086 (7) |
| N2 | 0.0453 (9) | 0.0410 (9) | 0.0558 (9) | −0.0032 (7) | 0.0156 (7) | −0.0043 (7) |
| C1 | 0.0423 (10) | 0.0366 (10) | 0.0481 (10) | −0.0005 (8) | 0.0095 (8) | −0.0007 (8) |
| C2 | 0.0474 (10) | 0.0364 (10) | 0.0545 (11) | 0.0001 (8) | 0.0126 (9) | −0.0029 (8) |
| C3 | 0.0445 (10) | 0.0431 (11) | 0.0530 (11) | −0.0042 (8) | 0.0072 (8) | 0.0024 (8) |
| C4 | 0.0403 (10) | 0.0556 (12) | 0.0666 (12) | −0.0026 (9) | 0.0145 (9) | −0.0033 (10) |
| C5 | 0.0450 (11) | 0.0503 (12) | 0.0686 (13) | 0.0014 (9) | 0.0146 (9) | −0.0131 (10) |
| C6 | 0.0419 (10) | 0.0385 (10) | 0.0519 (10) | 0.0004 (8) | 0.0072 (8) | −0.0039 (8) |
| C7 | 0.0449 (10) | 0.0394 (10) | 0.0448 (10) | −0.0021 (8) | 0.0074 (8) | −0.0016 (8) |
| C8 | 0.0459 (10) | 0.0433 (11) | 0.0446 (9) | −0.0058 (8) | 0.0095 (8) | −0.0043 (8) |
| C9 | 0.0587 (13) | 0.0506 (12) | 0.0579 (12) | −0.0065 (10) | 0.0043 (10) | 0.0044 (9) |
| C10 | 0.0820 (17) | 0.0535 (13) | 0.0625 (13) | −0.0223 (12) | 0.0088 (12) | 0.0089 (10) |
| C11 | 0.0623 (14) | 0.0713 (16) | 0.0702 (14) | −0.0285 (12) | 0.0205 (11) | −0.0040 (12) |
| C12 | 0.0474 (13) | 0.0732 (16) | 0.0897 (17) | −0.0075 (11) | 0.0139 (11) | −0.0017 (13) |
| C13 | 0.0524 (12) | 0.0505 (12) | 0.0731 (14) | −0.0045 (10) | 0.0143 (10) | 0.0022 (10) |
| C14 | 0.0500 (12) | 0.0478 (12) | 0.0613 (12) | −0.0066 (9) | 0.0099 (10) | 0.0027 (9) |
| C15 | 0.0873 (18) | 0.0516 (14) | 0.1029 (19) | −0.0304 (13) | 0.0256 (15) | −0.0133 (13) |
| C16 | 0.109 (2) | 0.0612 (16) | 0.123 (2) | −0.0270 (16) | 0.0293 (19) | −0.0215 (16) |
| C17 | 0.0572 (13) | 0.0468 (12) | 0.0804 (15) | −0.0078 (10) | 0.0197 (11) | −0.0239 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C18 | 0.0765 (18) | 0.095 (2) | 0.0720 (16) | −0.0237 (15) | 0.0244 (13) | −0.0351 (14) |
| C19 | 0.098 (2) | 0.114 (2) | 0.0592 (15) | −0.0281 (19) | 0.0050 (14) | 0.0001 (15) |
| C20 | 0.0765 (18) | 0.0528 (15) | 0.165 (3) | 0.0089 (13) | 0.0213 (18) | −0.0266 (16) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| F1—C11 | 1.359 (2) | C10—C11 | 1.363 (4) |
| O1—C14 | 1.207 (2) | C10—H10 | 0.9300 |
| O2—C14 | 1.329 (3) | C11—C12 | 1.355 (4) |
| O2—C15 | 1.451 (3) | C12—C13 | 1.382 (3) |
| N1—C7 | 1.383 (2) | C12—H12 | 0.9300 |
| N1—C6 | 1.384 (2) | C13—H13 | 0.9300 |
| N1—C17 | 1.480 (2) | C15—C16 | 1.456 (4) |
| N2—C7 | 1.315 (2) | C15—H15A | 0.9700 |
| N2—C1 | 1.391 (2) | C15—H15B | 0.9700 |
| C1—C2 | 1.390 (3) | C16—H16A | 0.9600 |
| C1—C6 | 1.396 (2) | C16—H16B | 0.9600 |
| C2—C3 | 1.387 (3) | C16—H16C | 0.9600 |
| C2—H2 | 0.9300 | C17—C18 | 1.506 (4) |
| C3—C4 | 1.397 (3) | C17—C20 | 1.549 (4) |
| C3—C14 | 1.474 (3) | C17—H17 | 0.9800 |
| C4—C5 | 1.372 (3) | C18—C19 | 1.468 (4) |
| C4—H4 | 0.9300 | C18—H18A | 0.9700 |
| C5—C6 | 1.396 (3) | C18—H18B | 0.9700 |
| C5—H5 | 0.9300 | C19—H19A | 0.9600 |
| C7—C8 | 1.473 (3) | C19—H19B | 0.9600 |
| C8—C13 | 1.379 (3) | C19—H19C | 0.9600 |
| C8—C9 | 1.393 (3) | C20—H20A | 0.9600 |
| C9—C10 | 1.376 (3) | C20—H20B | 0.9600 |
| C9—H9 | 0.9300 | C20—H20C | 0.9600 |
| C14—O2—C15 | 116.83 (18) | C8—C13—H13 | 119.4 |
| C7—N1—C6 | 105.97 (14) | C12—C13—H13 | 119.4 |
| C7—N1—C17 | 126.27 (16) | O1—C14—O2 | 122.46 (19) |
| C6—N1—C17 | 125.85 (16) | O1—C14—C3 | 124.7 (2) |
| C7—N2—C1 | 104.55 (15) | O2—C14—C3 | 112.79 (17) |
| C2—C1—N2 | 129.17 (16) | O2—C15—C16 | 107.4 (2) |
| C2—C1—C6 | 120.37 (17) | O2—C15—H15A | 110.2 |
| N2—C1—C6 | 110.45 (15) | C16—C15—H15A | 110.2 |
| C3—C2—C1 | 118.30 (17) | O2—C15—H15B | 110.2 |
| C3—C2—H2 | 120.8 | C16—C15—H15B | 110.2 |
| C1—C2—H2 | 120.9 | H15A—C15—H15B | 108.5 |
| C2—C3—C4 | 120.33 (18) | C15—C16—H16A | 109.5 |
| C2—C3—C14 | 121.51 (18) | C15—C16—H16B | 109.5 |
| C4—C3—C14 | 118.15 (18) | H16A—C16—H16B | 109.5 |
| C5—C4—C3 | 122.36 (19) | C15—C16—H16C | 109.5 |
| C5—C4—H4 | 118.8 | H16A—C16—H16C | 109.5 |
| C3—C4—H4 | 118.8 | H16B—C16—H16C | 109.5 |
| C4—C5—C6 | 116.93 (18) | N1—C17—C18 | 110.73 (18) |
| C4—C5—H5 | 121.5 | N1—C17—C20 | 110.4 (2) |

| | | | |
|---|---|---|---|
| C6—C5—H5 | 121.5 | C18—C17—C20 | 114.4 (2) |
| N1—C6—C1 | 105.64 (16) | N1—C17—H17 | 106.9 |
| N1—C6—C5 | 132.65 (17) | C18—C17—H17 | 106.9 |
| C1—C6—C5 | 121.70 (17) | C20—C17—H17 | 106.9 |
| N2—C7—N1 | 113.38 (16) | C19—C18—C17 | 112.7 (2) |
| N2—C7—C8 | 122.88 (16) | C19—C18—H18A | 109.1 |
| N1—C7—C8 | 123.72 (16) | C17—C18—H18A | 109.1 |
| C13—C8—C9 | 118.32 (18) | C19—C18—H18B | 109.1 |
| C13—C8—C7 | 119.53 (18) | C17—C18—H18B | 109.1 |
| C9—C8—C7 | 122.07 (18) | H18A—C18—H18B | 107.8 |
| C10—C9—C8 | 120.8 (2) | C18—C19—H19A | 109.5 |
| C10—C9—H9 | 119.6 | C18—C19—H19B | 109.5 |
| C8—C9—H9 | 119.6 | H19A—C19—H19B | 109.5 |
| C11—C10—C9 | 118.5 (2) | C18—C19—H19C | 109.5 |
| C11—C10—H10 | 120.8 | H19A—C19—H19C | 109.5 |
| C9—C10—H10 | 120.8 | H19B—C19—H19C | 109.5 |
| C12—C11—F1 | 118.7 (2) | C17—C20—H20A | 109.5 |
| C12—C11—C10 | 122.9 (2) | C17—C20—H20B | 109.5 |
| F1—C11—C10 | 118.4 (2) | H20A—C20—H20B | 109.5 |
| C11—C12—C13 | 118.3 (2) | C17—C20—H20C | 109.5 |
| C11—C12—H12 | 120.9 | H20A—C20—H20C | 109.5 |
| C13—C12—H12 | 120.9 | H20B—C20—H20C | 109.5 |
| C8—C13—C12 | 121.2 (2) | | |

| | | | |
|---|---|---|---|
| C7—N2—C1—C2 | 179.31 (19) | N1—C7—C8—C13 | 138.2 (2) |
| C7—N2—C1—C6 | −0.2 (2) | N2—C7—C8—C9 | 133.3 (2) |
| N2—C1—C2—C3 | 179.81 (18) | N1—C7—C8—C9 | −45.0 (3) |
| C6—C1—C2—C3 | −0.7 (3) | C13—C8—C9—C10 | −0.4 (3) |
| C1—C2—C3—C4 | 0.4 (3) | C7—C8—C9—C10 | −177.26 (18) |
| C1—C2—C3—C14 | −178.35 (17) | C8—C9—C10—C11 | 0.1 (3) |
| C2—C3—C4—C5 | 0.3 (3) | C9—C10—C11—C12 | 0.6 (4) |
| C14—C3—C4—C5 | 179.11 (19) | C9—C10—C11—F1 | −179.65 (19) |
| C3—C4—C5—C6 | −0.7 (3) | F1—C11—C12—C13 | 179.3 (2) |
| C7—N1—C6—C1 | 0.10 (19) | C10—C11—C12—C13 | −0.9 (4) |
| C17—N1—C6—C1 | −164.91 (18) | C9—C8—C13—C12 | 0.1 (3) |
| C7—N1—C6—C5 | −179.7 (2) | C7—C8—C13—C12 | 176.99 (19) |
| C17—N1—C6—C5 | 15.3 (3) | C11—C12—C13—C8 | 0.6 (3) |
| C2—C1—C6—N1 | −179.50 (16) | C15—O2—C14—O1 | −1.0 (3) |
| N2—C1—C6—N1 | 0.1 (2) | C15—O2—C14—C3 | 179.5 (2) |
| C2—C1—C6—C5 | 0.3 (3) | C2—C3—C14—O1 | 177.9 (2) |
| N2—C1—C6—C5 | 179.88 (18) | C4—C3—C14—O1 | −1.0 (3) |
| C4—C5—C6—N1 | −179.9 (2) | C2—C3—C14—O2 | −2.6 (3) |
| C4—C5—C6—C1 | 0.4 (3) | C4—C3—C14—O2 | 178.55 (18) |
| C1—N2—C7—N1 | 0.3 (2) | C14—O2—C15—C16 | 170.5 (2) |
| C1—N2—C7—C8 | −178.22 (16) | C7—N1—C17—C18 | −110.7 (2) |
| C6—N1—C7—N2 | −0.2 (2) | C6—N1—C17—C18 | 51.3 (3) |
| C17—N1—C7—N2 | 164.68 (18) | C7—N1—C17—C20 | 121.5 (2) |
| C6—N1—C7—C8 | 178.24 (17) | C6—N1—C17—C20 | −76.5 (3) |
| C17—N1—C7—C8 | −16.8 (3) | N1—C17—C18—C19 | 50.7 (3) |
| N2—C7—C8—C13 | −43.5 (3) | C20—C17—C18—C19 | 176.3 (2) |

*Hydrogen-bond geometry (Å, °)*

*Cg*1 is the centroid of the N1/C7/N2/C1/C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5···O1$^{i}$ | 0.93 | 2.53 | 3.452 (3) | 169 |
| C20—H20C···O1$^{i}$ | 0.96 | 2.59 | 3.485 (4) | 154 |
| C19—H19A···Cg1 | 0.96 | 2.82 | 3.400 (3) | 121 |

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

Fig. 1

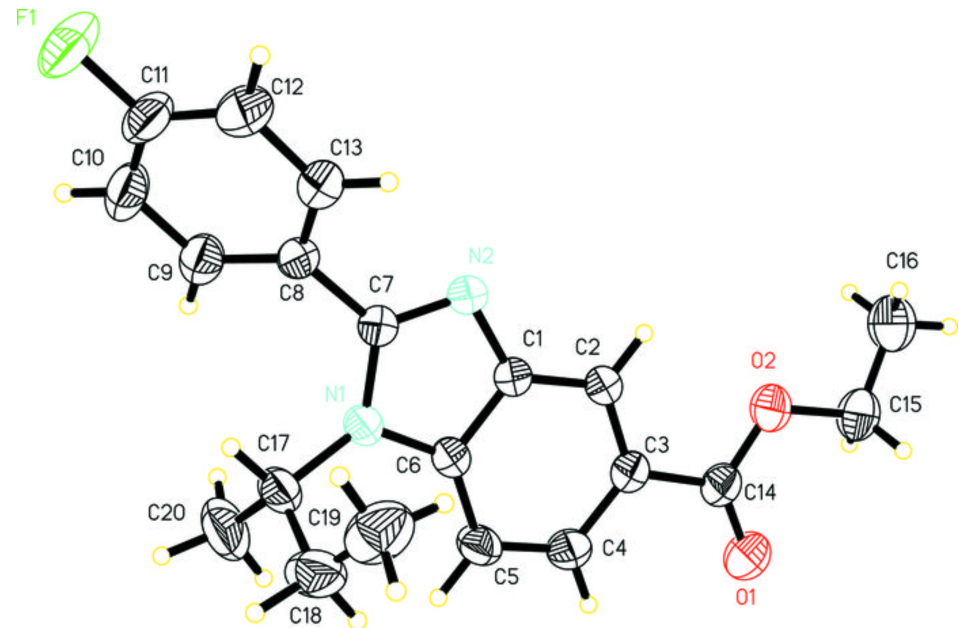
F1
C11
C12
C10
C13
C9
C8
C7
N2
C16
C1
C2
O2
N1
C15
C17
C6
C3
C14
C20
C19
C5
C4
C18
O1

Fig. 2