Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Sai Bi,[a] Hao Luo,[a] Wu-Lan Zeng[b] and Jun Wan[a]*

[a]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China, and [b]Department of Chemistry and Chemical Engineering, Weifang University, 261061 Weifang, Shandong, People's Republic of China
Correspondence e-mail: qustchemistry@126.com

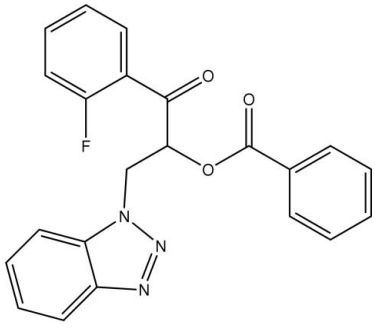
Received 21 October 2007; accepted 25 October 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.118; data-to-parameter ratio = 13.8.

In the molecule of the title compound, $C_{22}H_{16}FN_3O_3$, intramolecular C—H···F hydrogen bonding results in the formation of a six-membered ring. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules into centrosymmetric dimers. The packing is further stabilized by π–π interactions [centroid–centroid distance = 3.601 (2) Å].

Related literature

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



Experimental

Crystal data

$C_{22}H_{16}FN_3O_3$
M_r = 389.38
Triclinic, $P\overline{1}$
a = 9.8372 (11) Å
b = 9.8985 (12) Å
c = 11.6126 (13) Å
α = 115.187 (2)°
β = 101.572 (2)°
γ = 103.929 (2)°
V = 932.17 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.32 × 0.25 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.990
5309 measured reflections
3612 independent reflections
2543 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.118
S = 1.04
3612 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3B···O3^{i}	0.93	2.53	3.375 (3)	152
C8—H8A···F1	0.98	2.27	2.753 (2)	110

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

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).

This project was supported by the Natural Science Foundation of Shandong Province (grant Nos. Z2006B01 and Y2006B07).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2350).

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.
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*. 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.
Wan, J., Zeng, W.-L., Li, J. & Bi, S. (2007). *Acta Cryst.* E**63**, o3949.

 doi:10.1107/S1600536807053251

supplementary materials

Acta Cryst. (2007). E**63**, o4499 [**doi:10.1107/S1600536807053251**]

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

S. Bi, H. Luo, W.-L. Zeng and J. Wan

Comment

We have recently reported the structure of 3-(1*H*-Benzotriazol-1-yl)-1 -(2-fluorobenzoyl)ethyl nicotinate, (II), (Wan *et al.*, 2007). As part of our ongoing studies to search for benzotriazole derivatives with higher pharmacological activities, such as antifungal, antitumor and antineoplastic, the title compound (I) was synthesized and its crystal structure is reported here.

In the molecule of the title compound, (I), (Fig. 1) 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 group is essentially planar, with a dihedral angle of 0.99 (1)° between triazole A (N1—N3/C10/C11) and benzene B (C10—C15) rings. Rings C (C1—C6) and D (C17—C22) are oriented with respect to the benzotriazole system at dihedral angles of 3.22 (1) and 86.48 (1)°, respectively, while the dihedral angle between them is 88.08 (1)°. The intramolecular C—H···F hydrogen bond (Table 1) results in the formation of a six-membered ring E (F1/C1/C6—C8/H8A) (Fig. 1).

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 1), link the molecules into centrosymmetric dimers (Fig. 2). The packing is further stabilized by π-π interactions involving the C rings with centroid-centroid distance of 3.601 (2) Å (symmetry code: 1 − *x*, −*y*, −*z*).

Experimental

The title compound was prepared according to the literature method (Wan *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

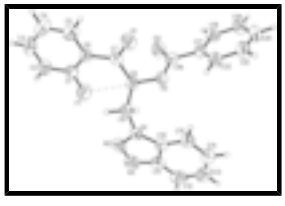


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

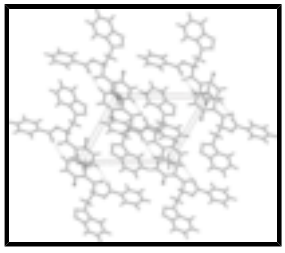


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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

Crystal data

$C_{22}H_{16}FN_3O_3$	$Z = 2$
$M_r = 389.38$	$F_{000} = 404$
Triclinic, $P\bar{1}$	$D_x = 1.387$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.8372$ (11) Å	Cell parameters from 1186 reflections
$b = 9.8985$ (12) Å	$\theta = 2.3$–24.9°
$c = 11.6126$ (13) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 115.187$ (2)°	$T = 294$ (2) K
$\beta = 101.572$ (2)°	Block, colorless
$\gamma = 103.929$ (2)°	0.32 × 0.25 × 0.10 mm
$V = 932.17$ (19) Å^3	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3612 independent reflections
Radiation source: fine-focus sealed tube	2543 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.019$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.0^\circ$
$T = 294(2)$ K	$\theta_{min} = 2.1^\circ$
ω scans	$h = -12 \rightarrow 6$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -11 \rightarrow 12$
$T_{min} = 0.968$, $T_{max} = 0.990$	$l = -14 \rightarrow 14$
5309 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
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 0.1753P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
3612 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.20$ 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	0.60239 (17)	0.34447 (16)	0.07729 (12)	0.0707 (4)
O1	0.84080 (18)	0.27597 (19)	0.37136 (14)	0.0602 (5)
O2	0.77177 (15)	0.52712 (15)	0.49177 (12)	0.0436 (4)
O3	0.55363 (18)	0.34154 (19)	0.44232 (15)	0.0614 (5)
N1	0.80939 (19)	0.72821 (19)	0.36119 (16)	0.0410 (4)
N2	0.7254 (2)	0.7301 (2)	0.25404 (17)	0.0536 (5)
N3	0.6900 (2)	0.8564 (2)	0.2985 (2)	0.0589 (5)
C1	0.6462 (2)	0.2172 (2)	0.0430 (2)	0.0443 (5)
C2	0.6046 (3)	0.1115 (3)	−0.0929 (2)	0.0562 (6)
H2B	0.5498	0.1285	−0.1572	0.067*
C3	0.6455 (3)	−0.0192 (3)	−0.1316 (2)	0.0629 (7)
H3B	0.6199	−0.0913	−0.2232	0.076*
C4	0.7243 (3)	−0.0447 (3)	−0.0359 (3)	0.0650 (7)
H4A	0.7508	−0.1345	−0.0628	0.078*
C5	0.7640 (2)	0.0628 (3)	0.0997 (2)	0.0535 (6)
H5A	0.8171	0.0440	0.1635	0.064*
C6	0.7269 (2)	0.1990 (2)	0.14382 (19)	0.0394 (5)
C7	0.7744 (2)	0.3082 (2)	0.2927 (2)	0.0400 (5)
C8	0.7447 (2)	0.4643 (2)	0.34929 (18)	0.0393 (5)
H8A	0.6418	0.4454	0.3018	0.047*
C9	0.8546 (2)	0.5926 (2)	0.3385 (2)	0.0429 (5)
H9A	0.9523	0.6300	0.4046	0.051*
H9B	0.8627	0.5455	0.2491	0.051*
C10	0.8278 (2)	0.8585 (2)	0.4790 (2)	0.0404 (5)
C11	0.7505 (2)	0.9393 (3)	0.4378 (2)	0.0478 (5)
C12	0.7438 (3)	1.0812 (3)	0.5334 (3)	0.0659 (7)
H12A	0.6908	1.1357	0.5074	0.079*

C13	0.8184 (3)	1.1363 (3)	0.6665 (3)	0.0704 (8)
H13A	0.8162	1.2303	0.7326	0.084*
C14	0.8982 (3)	1.0544 (3)	0.7057 (2)	0.0656 (7)
H14A	0.9486	1.0969	0.7975	0.079*
C15	0.9049 (3)	0.9151 (3)	0.6149 (2)	0.0517 (6)
H15A	0.9577	0.8610	0.6419	0.062*
C16	0.6693 (2)	0.4465 (2)	0.5249 (2)	0.0411 (5)
C17	0.7187 (2)	0.5001 (2)	0.67165 (19)	0.0389 (5)
C18	0.6172 (3)	0.4414 (3)	0.7218 (2)	0.0485 (5)
H18A	0.5200	0.3731	0.6644	0.058*
C19	0.6600 (3)	0.4842 (3)	0.8570 (2)	0.0563 (6)
H19A	0.5907	0.4474	0.8911	0.068*
C20	0.8046 (3)	0.5809 (3)	0.9413 (2)	0.0594 (7)
H20A	0.8335	0.6077	1.0320	0.071*
C21	0.9073 (3)	0.6385 (3)	0.8918 (2)	0.0591 (7)
H21A	1.0054	0.7031	0.9487	0.071*
C22	0.8637 (2)	0.5997 (3)	0.7575 (2)	0.0477 (6)
H22A	0.9320	0.6407	0.7247	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1010 (12)	0.0678 (9)	0.0465 (8)	0.0491 (9)	0.0129 (8)	0.0272 (7)
O1	0.0772 (12)	0.0693 (11)	0.0448 (9)	0.0394 (9)	0.0157 (8)	0.0333 (8)
O2	0.0501 (9)	0.0428 (8)	0.0305 (7)	0.0095 (7)	0.0149 (7)	0.0156 (6)
O3	0.0550 (10)	0.0615 (10)	0.0442 (9)	0.0003 (9)	0.0100 (8)	0.0208 (8)
N1	0.0481 (11)	0.0417 (10)	0.0349 (9)	0.0158 (8)	0.0115 (8)	0.0221 (8)
N2	0.0615 (13)	0.0555 (12)	0.0443 (11)	0.0163 (10)	0.0099 (10)	0.0318 (10)
N3	0.0670 (14)	0.0561 (12)	0.0607 (13)	0.0234 (11)	0.0135 (11)	0.0385 (11)
C1	0.0469 (13)	0.0430 (12)	0.0423 (12)	0.0176 (10)	0.0144 (10)	0.0206 (10)
C2	0.0612 (16)	0.0571 (15)	0.0354 (12)	0.0134 (12)	0.0077 (11)	0.0189 (11)
C3	0.0614 (17)	0.0551 (15)	0.0396 (13)	0.0076 (13)	0.0142 (12)	0.0048 (12)
C4	0.0663 (17)	0.0458 (14)	0.0617 (16)	0.0232 (13)	0.0176 (14)	0.0097 (12)
C5	0.0505 (14)	0.0485 (13)	0.0527 (14)	0.0200 (11)	0.0102 (11)	0.0202 (11)
C6	0.0392 (12)	0.0393 (11)	0.0360 (11)	0.0121 (9)	0.0124 (10)	0.0172 (9)
C7	0.0398 (12)	0.0466 (12)	0.0384 (11)	0.0155 (10)	0.0141 (10)	0.0250 (10)
C8	0.0455 (13)	0.0423 (11)	0.0283 (10)	0.0165 (10)	0.0113 (9)	0.0165 (9)
C9	0.0496 (13)	0.0453 (12)	0.0383 (11)	0.0206 (10)	0.0180 (10)	0.0218 (10)
C10	0.0432 (13)	0.0375 (11)	0.0416 (12)	0.0126 (9)	0.0158 (10)	0.0214 (10)
C11	0.0514 (14)	0.0443 (12)	0.0546 (14)	0.0170 (11)	0.0182 (12)	0.0307 (11)
C12	0.0767 (19)	0.0538 (15)	0.089 (2)	0.0355 (14)	0.0374 (17)	0.0444 (15)
C13	0.095 (2)	0.0457 (14)	0.0719 (18)	0.0292 (14)	0.0408 (17)	0.0230 (13)
C14	0.085 (2)	0.0522 (15)	0.0460 (14)	0.0197 (14)	0.0195 (14)	0.0173 (12)
C15	0.0594 (15)	0.0481 (13)	0.0426 (13)	0.0196 (11)	0.0128 (11)	0.0206 (11)
C16	0.0450 (13)	0.0389 (11)	0.0394 (12)	0.0164 (10)	0.0160 (11)	0.0184 (10)
C17	0.0471 (13)	0.0373 (11)	0.0368 (11)	0.0195 (10)	0.0193 (10)	0.0180 (9)
C18	0.0496 (14)	0.0516 (13)	0.0489 (13)	0.0172 (11)	0.0212 (11)	0.0278 (11)
C19	0.0693 (17)	0.0629 (15)	0.0532 (14)	0.0263 (13)	0.0347 (13)	0.0360 (13)

C20	0.0771 (19)	0.0663 (16)	0.0370 (12)	0.0259 (14)	0.0235 (13)	0.0262 (12)
C21	0.0568 (16)	0.0672 (16)	0.0402 (13)	0.0143 (13)	0.0119 (12)	0.0223 (12)
C22	0.0501 (14)	0.0516 (13)	0.0416 (12)	0.0162 (11)	0.0214 (11)	0.0223 (11)

Geometric parameters (Å, °)

O2—C16	1.352 (2)	C22—C21	1.380 (3)
O2—C8	1.436 (2)	C22—H22A	0.9300
F1—C1	1.354 (2)	C18—C19	1.380 (3)
O3—C16	1.200 (2)	C18—H18A	0.9300
N1—N2	1.359 (2)	C19—C20	1.373 (3)
N1—C10	1.362 (2)	C19—H19A	0.9300
N1—C9	1.450 (2)	C5—C4	1.375 (3)
O1—C7	1.213 (2)	C5—H5A	0.9300
C17—C22	1.384 (3)	C11—C12	1.399 (3)
C17—C18	1.385 (3)	C2—C3	1.366 (3)
C17—C16	1.482 (3)	C2—H2B	0.9300
N3—N2	1.297 (2)	C21—C20	1.382 (3)
N3—C11	1.375 (3)	C21—H21A	0.9300
C6—C1	1.382 (3)	C20—H20A	0.9300
C6—C5	1.391 (3)	C3—C4	1.373 (3)
C6—C7	1.489 (3)	C3—H3B	0.9300
C8—C9	1.525 (3)	C4—H4A	0.9300
C8—C7	1.529 (3)	C14—C15	1.361 (3)
C8—H8A	0.9800	C14—C13	1.400 (3)
C9—H9A	0.9700	C14—H14A	0.9300
C9—H9B	0.9700	C15—H15A	0.9300
C1—C2	1.371 (3)	C12—C13	1.363 (3)
C10—C11	1.386 (3)	C12—H12A	0.9300
C10—C15	1.394 (3)	C13—H13A	0.9300
C16—O2—C8	115.86 (15)	C19—C18—C17	120.1 (2)
N2—N1—C10	109.85 (17)	C19—C18—H18A	120.0
N2—N1—C9	119.67 (16)	C17—C18—H18A	120.0
C10—N1—C9	130.29 (17)	C20—C19—C18	120.2 (2)
C22—C17—C18	119.53 (19)	C20—C19—H19A	119.9
C22—C17—C16	122.21 (18)	C18—C19—H19A	119.9
C18—C17—C16	118.19 (19)	C4—C5—C6	121.7 (2)
N2—N3—C11	108.13 (18)	C4—C5—H5A	119.2
C1—C6—C5	115.72 (19)	C6—C5—H5A	119.2
C1—C6—C7	126.45 (19)	N3—C11—C10	108.78 (19)
C5—C6—C7	117.82 (19)	N3—C11—C12	130.8 (2)
O2—C8—C9	105.53 (15)	C10—C11—C12	120.4 (2)
O2—C8—C7	109.03 (15)	C3—C2—C1	118.5 (2)
C9—C8—C7	110.79 (16)	C3—C2—H2B	120.8
O2—C8—H8A	110.5	C1—C2—H2B	120.8
C9—C8—H8A	110.5	C22—C21—C20	119.8 (2)
C7—C8—H8A	110.5	C22—C21—H21A	120.1
N3—N2—N1	109.04 (17)	C20—C21—H21A	120.1
O3—C16—O2	122.66 (18)	C19—C20—C21	120.2 (2)

O3—C16—C17	124.95 (19)	C19—C20—H20A	119.9
O2—C16—C17	112.38 (18)	C21—C20—H20A	119.9
O1—C7—C6	120.20 (19)	C2—C3—C4	120.4 (2)
O1—C7—C8	118.75 (18)	C2—C3—H3B	119.8
C6—C7—C8	121.03 (17)	C4—C3—H3B	119.8
N1—C9—C8	112.24 (17)	C3—C4—C5	120.0 (2)
N1—C9—H9A	109.2	C3—C4—H4A	120.0
C8—C9—H9A	109.2	C5—C4—H4A	120.0
N1—C9—H9B	109.2	C15—C14—C13	122.6 (2)
C8—C9—H9B	109.2	C15—C14—H14A	118.7
H9A—C9—H9B	107.9	C13—C14—H14A	118.7
F1—C1—C2	116.7 (2)	C14—C15—C10	115.8 (2)
F1—C1—C6	119.51 (18)	C14—C15—H15A	122.1
C2—C1—C6	123.8 (2)	C10—C15—H15A	122.1
N1—C10—C11	104.19 (17)	C13—C12—C11	117.2 (2)
N1—C10—C15	133.3 (2)	C13—C12—H12A	121.4
C11—C10—C15	122.5 (2)	C11—C12—H12A	121.4
C21—C22—C17	120.2 (2)	C12—C13—C14	121.4 (2)
C21—C22—H22A	119.9	C12—C13—H13A	119.3
C17—C22—H22A	119.9	C14—C13—H13A	119.3
C16—O2—C8—C9	168.65 (16)	C9—N1—C10—C15	6.6 (4)
C16—O2—C8—C7	−72.3 (2)	C18—C17—C22—C21	1.0 (3)
C11—N3—N2—N1	−0.5 (2)	C16—C17—C22—C21	−175.9 (2)
C10—N1—N2—N3	0.3 (2)	C22—C17—C18—C19	0.9 (3)
C9—N1—N2—N3	175.79 (17)	C16—C17—C18—C19	177.9 (2)
C8—O2—C16—O3	−8.9 (3)	C17—C18—C19—C20	−2.0 (3)
C8—O2—C16—C17	169.57 (16)	C1—C6—C5—C4	1.0 (3)
C22—C17—C16—O3	167.6 (2)	C7—C6—C5—C4	179.8 (2)
C18—C17—C16—O3	−9.3 (3)	N2—N3—C11—C10	0.6 (2)
C22—C17—C16—O2	−10.9 (3)	N2—N3—C11—C12	−179.3 (2)
C18—C17—C16—O2	172.22 (18)	N1—C10—C11—N3	−0.4 (2)
C1—C6—C7—O1	177.4 (2)	C15—C10—C11—N3	178.39 (19)
C5—C6—C7—O1	−1.3 (3)	N1—C10—C11—C12	179.50 (19)
C1—C6—C7—C8	−4.3 (3)	C15—C10—C11—C12	−1.7 (3)
C5—C6—C7—C8	177.00 (18)	F1—C1—C2—C3	−179.4 (2)
O2—C8—C7—O1	−14.0 (3)	C6—C1—C2—C3	−0.3 (4)
C9—C8—C7—O1	101.7 (2)	C17—C22—C21—C20	−1.7 (4)
O2—C8—C7—C6	167.59 (17)	C18—C19—C20—C21	1.3 (4)
C9—C8—C7—C6	−76.7 (2)	C22—C21—C20—C19	0.6 (4)
N2—N1—C9—C8	−92.3 (2)	C1—C2—C3—C4	1.1 (4)
C10—N1—C9—C8	82.1 (3)	C2—C3—C4—C5	−0.8 (4)
O2—C8—C9—N1	−75.6 (2)	C6—C5—C4—C3	−0.3 (4)
C7—C8—C9—N1	166.56 (16)	C13—C14—C15—C10	0.4 (4)
C5—C6—C1—F1	178.43 (18)	N1—C10—C15—C14	179.2 (2)
C7—C6—C1—F1	−0.3 (3)	C11—C10—C15—C14	0.9 (3)
C5—C6—C1—C2	−0.7 (3)	N3—C11—C12—C13	−178.9 (2)
C7—C6—C1—C2	−179.5 (2)	C10—C11—C12—C13	1.2 (3)
N2—N1—C10—C11	0.1 (2)	C11—C12—C13—C14	0.0 (4)
C9—N1—C10—C11	−174.82 (18)	C15—C14—C13—C12	−0.9 (4)

N2—N1—C10—C15	−178.5 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3B···O3^{i}	0.93	2.53	3.375 (3)	152
C8—H8A···F1	0.98	2.27	2.753 (2)	110

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

Fig. 1

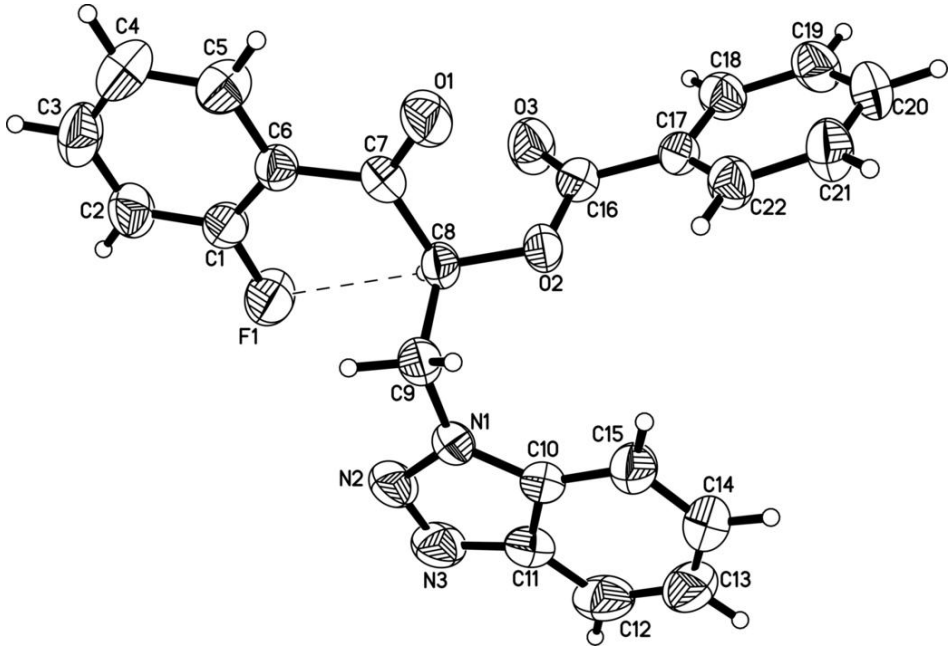

C4
C5
C3
C6
C7
O1
O3
C17
C18
C19
C20
C21
C22
C16
C2
C1
C8
O2
F1
C9
N1
C10
C15
N2
C14
N3
C11
C13
C12

Fig. 2