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3-(1*H*-Benzotriazol-1-yl)-1-(4-fluorobenzoyl)ethyl benzoate

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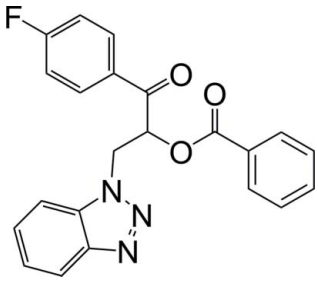
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.130; data-to-parameter ratio = 12.7.

In the crystal structure of the title compound, $C_{22}H_{16}FN_3O_3$, weak intermolecular C—H···O hydrogen bonds link the molecules into chains extending along the C axis. The packing is further stabilized by weak C—H···π interactions.

Related literature

For background, see Chen & Wu (2005). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{16}FN_3O_3$
M_r = 389.38
Monoclinic, $P2_1/c$
a = 10.302 (10) Å
b = 9.089 (9) Å
c = 20.38 (2) Å
β = 99.687 (18)°
V = 1881 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.978, T_{max} = 0.990
9421 measured reflections
3322 independent reflections
1791 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.130
S = 1.01
3322 reflections
262 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

Cg is the centroid of the N1–N3/C10/C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.59	3.292 (5)	133
C8—H8···O1^{i}	0.98	2.50	3.470 (5)	173
C9—H9A···O3^{ii}	0.97	2.34	3.057 (4)	130
C1—H1···Cg^{ii}	0.93	2.95	3.730 (5)	143

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2525).

References

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supplementary materials

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3-(1*H*-Benzotriazol-1-yl)-1-(4-fluorobenzoyl)ethyl benzoate

W.-L. Zeng

Comment

1*H*-Benzotriazole and its derivatives exhibit a broad spectrum of pharmacological activities such as antifungal, antitumor and antineoplastic activities (Chen & Wu, 2005). We report here the synthesis and structure of the title compound, (I) (Fig. 1), as part of our ongoing studies on new benzotriazole compounds with higher bioactivity.

All the bond lengths and angles in (I) are within their normal ranges (Allen *et al.*, 1987). The benzotriazole ring system is essentially planar, with a dihedral angle of 0.83 (1)° between the triazole ring (atoms N1–N3/C10/C15) and the C10–C15 benzene ring. The dihedral angles between the mean planes of the benzotriazole system and the C1–C6 and C17–C22 aromatic rings are 6.52 (1)° and 82.67 (1)°, respectively. The dihedral angle between rings C1–C6 and C17–C22 is 78.04 (2)°. In the arbitrarily chosen asymmetric molecule, atom C8 has *R* configuration, but crystal symmetry generates a racemic mixture.

In the crystal structure of (I), weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into chains extended along the *c* axis. The packing is further stabilized by weak C—H···π interactions.

Experimental

Bromine (3.2 g, 0.02 mol) was added dropwise to a solution of 3-(1*H*-benzo[*d*][1,2,3]triazol-1-yl)-1-(4-fluorophenyl)propan-1-one (5.38 g, 0.02 mol) and sodium acetate (1.6 g, 0.02 mol) in acetic acid (50 ml). The reaction proceeded for 7 h. Water (50 ml) and chloroform (20 ml) were then added. The organic layer was washed successively with saturated sodium bicarbonate solution and brine, dried over anhydrous magnesium sulfate and the chloroform solution filtered. It was cooled with ice–water, and then an acetone solution (10 ml) of benzoic acid (2.44 g, 0.02 mol) and triethylamine (2.8 ml) was added. The mixture was stirred with ice–water for 6 h. The solution was then filtered and concentrated. Colourless blocks of (I) were obtained by slow evaporation of an acetone–ethyl acetate (1:1 *v*/*v*) solution at room temperature over a period of one week.

Refinement

The H atoms were geometrically placed (C—H = 0.93–0.97 Å), and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

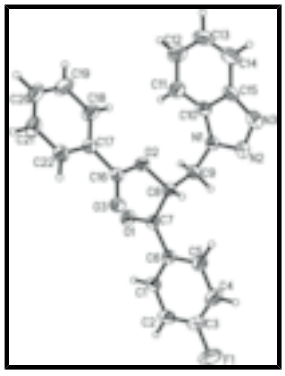


Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids (arbitrary spheres for the H atoms).

3-(1*H*-Benzotriazol-1-yl)-1-(4-fluorobenzoyl)ethyl benzoate

Crystal data

$C_{22}H_{16}FN_3O_3$	F_{000} = 808
M_r = 389.38	D_x = 1.375 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1779 reflections
a = 10.302 (10) Å	θ = 2.6–22.7º
b = 9.089 (9) Å	μ = 0.10 mm^{-1}
c = 20.38 (2) Å	T = 294 (2) K
β = 99.687 (18)º	Block, colourless
V = 1881 (3) Å^3	0.22 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3322 independent reflections
Radiation source: fine-focus sealed tube	1791 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.056
T = 294(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −12→12
T_{min} = 0.978, T_{max} = 0.990	k = −10→8
9421 measured reflections	l = −24→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
3322 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
F1	0.94092 (17)	0.1533 (3)	0.44908 (9)	0.1242 (8)
O1	0.39664 (16)	−0.0227 (2)	0.28432 (8)	0.0588 (5)
O2	0.31492 (14)	0.16117 (18)	0.18101 (7)	0.0469 (5)
O3	0.32855 (15)	0.30853 (19)	0.26935 (8)	0.0532 (5)
N1	0.48331 (19)	0.1106 (2)	0.08562 (9)	0.0496 (6)
N2	0.5827 (2)	0.1996 (3)	0.07466 (11)	0.0709 (7)
N3	0.5485 (3)	0.2671 (3)	0.01856 (12)	0.0819 (8)
C1	0.6228 (3)	0.0203 (3)	0.37736 (11)	0.0581 (8)
H1	0.5576	−0.0411	0.3885	0.070*
C2	0.7357 (3)	0.0418 (4)	0.42226 (13)	0.0745 (9)
H2	0.7476	−0.0034	0.4638	0.089*
C3	0.8298 (3)	0.1305 (4)	0.40478 (14)	0.0739 (9)
C4	0.8165 (3)	0.1986 (4)	0.34496 (14)	0.0747 (9)
H4	0.8830	0.2590	0.3346	0.090*
C5	0.7027 (2)	0.1770 (3)	0.29968 (13)	0.0574 (7)
H5	0.6924	0.2224	0.2582	0.069*
C6	0.6038 (2)	0.0881 (3)	0.31566 (11)	0.0430 (6)
C7	0.4792 (2)	0.0597 (3)	0.26952 (11)	0.0436 (6)
C8	0.4535 (2)	0.1342 (3)	0.20131 (10)	0.0431 (6)
H8	0.5019	0.2274	0.2032	0.052*
C9	0.4947 (2)	0.0355 (3)	0.14860 (11)	0.0526 (7)
H9A	0.5851	0.0044	0.1627	0.063*
H9B	0.4396	−0.0517	0.1434	0.063*

C10	0.3811 (2)	0.1219 (3)	0.03451 (11)	0.0517 (7)
C11	0.2580 (3)	0.0561 (3)	0.02138 (14)	0.0711 (9)
H11	0.2302	−0.0128	0.0498	0.085*
C12	0.1798 (3)	0.1005 (5)	−0.03694 (17)	0.0938 (12)
H12	0.0955	0.0615	−0.0482	0.113*
C13	0.2236 (4)	0.2020 (5)	−0.07940 (15)	0.1014 (13)
H13	0.1674	0.2280	−0.1183	0.122*
C14	0.3428 (4)	0.2638 (4)	−0.06664 (14)	0.0909 (11)
H14	0.3702	0.3315	−0.0957	0.109*
C15	0.4241 (3)	0.2226 (3)	−0.00807 (12)	0.0633 (8)
C16	0.2639 (2)	0.2577 (3)	0.22011 (11)	0.0420 (6)
C17	0.1242 (2)	0.2922 (3)	0.19600 (11)	0.0451 (6)
C18	0.0535 (3)	0.2316 (3)	0.13901 (13)	0.0731 (9)
H18	0.0937	0.1652	0.1140	0.088*
C19	−0.0769 (3)	0.2694 (4)	0.11903 (15)	0.0917 (11)
H19	−0.1243	0.2284	0.0805	0.110*
C20	−0.1362 (3)	0.3655 (4)	0.15498 (16)	0.0776 (9)
H20	−0.2243	0.3897	0.1414	0.093*
C21	−0.0677 (3)	0.4266 (4)	0.21063 (15)	0.0718 (9)
H21	−0.1088	0.4935	0.2349	0.086*
C22	0.0624 (2)	0.3907 (3)	0.23167 (12)	0.0582 (7)
H22	0.1087	0.4332	0.2701	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0861 (13)	0.177 (2)	0.0929 (12)	−0.0360 (14)	−0.0312 (11)	0.0036 (13)
O1	0.0515 (10)	0.0589 (13)	0.0657 (11)	−0.0106 (10)	0.0090 (9)	0.0108 (10)
O2	0.0415 (9)	0.0508 (12)	0.0469 (9)	0.0075 (8)	0.0031 (7)	−0.0072 (8)
O3	0.0537 (10)	0.0575 (13)	0.0471 (10)	−0.0039 (9)	0.0049 (8)	−0.0114 (9)
N1	0.0454 (12)	0.0618 (16)	0.0429 (11)	0.0074 (11)	0.0108 (10)	0.0017 (11)
N2	0.0561 (14)	0.097 (2)	0.0633 (15)	−0.0029 (14)	0.0204 (12)	0.0056 (15)
N3	0.0809 (19)	0.106 (2)	0.0638 (15)	−0.0046 (16)	0.0251 (14)	0.0170 (16)
C1	0.0610 (17)	0.068 (2)	0.0448 (14)	−0.0075 (14)	0.0080 (13)	0.0028 (14)
C2	0.077 (2)	0.099 (3)	0.0440 (15)	−0.0052 (19)	−0.0001 (15)	0.0075 (17)
C3	0.0587 (18)	0.096 (3)	0.0601 (18)	−0.0087 (18)	−0.0102 (15)	−0.0058 (18)
C4	0.0537 (17)	0.084 (2)	0.083 (2)	−0.0153 (16)	−0.0003 (15)	0.0078 (19)
C5	0.0504 (16)	0.063 (2)	0.0584 (15)	0.0008 (15)	0.0073 (13)	0.0114 (15)
C6	0.0423 (14)	0.0426 (16)	0.0450 (14)	0.0004 (12)	0.0099 (11)	−0.0013 (13)
C7	0.0405 (14)	0.0415 (16)	0.0501 (14)	0.0037 (12)	0.0110 (11)	−0.0040 (13)
C8	0.0391 (13)	0.0444 (16)	0.0453 (13)	0.0061 (12)	0.0057 (11)	0.0004 (12)
C9	0.0535 (15)	0.0586 (19)	0.0461 (14)	0.0164 (13)	0.0093 (12)	0.0050 (14)
C10	0.0538 (16)	0.0589 (19)	0.0429 (14)	0.0141 (14)	0.0094 (13)	−0.0100 (14)
C11	0.0649 (19)	0.083 (2)	0.0644 (18)	0.0010 (17)	0.0082 (15)	−0.0143 (17)
C12	0.070 (2)	0.135 (4)	0.071 (2)	0.006 (2)	−0.0037 (19)	−0.031 (2)
C13	0.099 (3)	0.157 (4)	0.0454 (18)	0.038 (3)	0.0023 (19)	−0.001 (2)
C14	0.102 (3)	0.118 (3)	0.0538 (19)	0.029 (2)	0.0181 (18)	0.016 (2)
C15	0.072 (2)	0.079 (2)	0.0414 (15)	0.0200 (17)	0.0172 (14)	0.0067 (16)

C16	0.0469 (14)	0.0382 (16)	0.0423 (13)	0.0013 (12)	0.0114 (12)	0.0013 (13)
C17	0.0451 (14)	0.0451 (16)	0.0458 (13)	0.0008 (12)	0.0098 (11)	0.0001 (13)
C18	0.0512 (17)	0.091 (2)	0.0729 (18)	0.0159 (16)	−0.0013 (14)	−0.0283 (18)
C19	0.0537 (18)	0.126 (3)	0.087 (2)	0.021 (2)	−0.0109 (16)	−0.036 (2)
C20	0.0441 (16)	0.093 (3)	0.094 (2)	0.0149 (17)	0.0089 (16)	−0.004 (2)
C21	0.0556 (18)	0.072 (2)	0.092 (2)	0.0141 (16)	0.0238 (16)	−0.0106 (18)
C22	0.0573 (17)	0.061 (2)	0.0580 (15)	0.0033 (15)	0.0148 (13)	−0.0084 (15)

Geometric parameters (Å, °)

F1—C3	1.349 (3)	C9—H9A	0.9700
O1—C7	1.209 (3)	C9—H9B	0.9700
O2—C16	1.350 (3)	C10—C15	1.384 (4)
O2—C8	1.439 (3)	C10—C11	1.387 (4)
O3—C16	1.200 (3)	C11—C12	1.379 (4)
N1—N2	1.353 (3)	C11—H11	0.9300
N1—C10	1.355 (3)	C12—C13	1.391 (5)
N1—C9	1.441 (3)	C12—H12	0.9300
N2—N3	1.293 (3)	C13—C14	1.336 (5)
N3—C15	1.366 (4)	C13—H13	0.9300
C1—C2	1.368 (4)	C14—C15	1.389 (4)
C1—C6	1.384 (3)	C14—H14	0.9300
C1—H1	0.9300	C16—C17	1.474 (3)
C2—C3	1.354 (4)	C17—C22	1.375 (3)
C2—H2	0.9300	C17—C18	1.378 (3)
C3—C4	1.353 (4)	C18—C19	1.380 (4)
C4—C5	1.379 (3)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.351 (4)
C5—C6	1.381 (3)	C19—H19	0.9300
C5—H5	0.9300	C20—C21	1.350 (4)
C6—C7	1.481 (3)	C20—H20	0.9300
C7—C8	1.529 (3)	C21—C22	1.377 (4)
C8—C9	1.514 (3)	C21—H21	0.9300
C8—H8	0.9800	C22—H22	0.9300
C16—O2—C8	114.01 (17)	N1—C10—C15	104.0 (2)
N2—N1—C10	109.9 (2)	N1—C10—C11	133.1 (3)
N2—N1—C9	118.7 (2)	C15—C10—C11	122.9 (3)
C10—N1—C9	131.1 (2)	C12—C11—C10	115.0 (3)
N3—N2—N1	109.2 (2)	C12—C11—H11	122.5
N2—N3—C15	108.0 (2)	C10—C11—H11	122.5
C2—C1—C6	121.2 (3)	C11—C12—C13	121.8 (3)
C2—C1—H1	119.4	C11—C12—H12	119.1
C6—C1—H1	119.4	C13—C12—H12	119.1
C3—C2—C1	118.4 (3)	C14—C13—C12	122.8 (3)
C3—C2—H2	120.8	C14—C13—H13	118.6
C1—C2—H2	120.8	C12—C13—H13	118.6
F1—C3—C4	118.6 (3)	C13—C14—C15	117.1 (3)
F1—C3—C2	118.7 (3)	C13—C14—H14	121.5
C4—C3—C2	122.7 (3)	C15—C14—H14	121.5

C3—C4—C5	118.9 (3)	N3—C15—C10	108.9 (2)
C3—C4—H4	120.5	N3—C15—C14	130.6 (3)
C5—C4—H4	120.5	C10—C15—C14	120.4 (3)
C4—C5—C6	120.2 (2)	O3—C16—O2	121.8 (2)
C4—C5—H5	119.9	O3—C16—C17	124.8 (2)
C6—C5—H5	119.9	O2—C16—C17	113.4 (2)
C5—C6—C1	118.5 (2)	C22—C17—C18	118.7 (2)
C5—C6—C7	123.2 (2)	C22—C17—C16	118.4 (2)
C1—C6—C7	118.3 (2)	C18—C17—C16	122.9 (2)
O1—C7—C6	121.4 (2)	C17—C18—C19	119.9 (3)
O1—C7—C8	118.6 (2)	C17—C18—H18	120.0
C6—C7—C8	120.0 (2)	C19—C18—H18	120.0
O2—C8—C9	106.25 (17)	C20—C19—C18	120.5 (3)
O2—C8—C7	110.42 (18)	C20—C19—H19	119.7
C9—C8—C7	110.9 (2)	C18—C19—H19	119.7
O2—C8—H8	109.8	C21—C20—C19	120.1 (3)
C9—C8—H8	109.8	C21—C20—H20	119.9
C7—C8—H8	109.7	C19—C20—H20	119.9
N1—C9—C8	111.1 (2)	C20—C21—C22	120.5 (3)
N1—C9—H9A	109.4	C20—C21—H21	119.7
C8—C9—H9A	109.4	C22—C21—H21	119.7
N1—C9—H9B	109.4	C17—C22—C21	120.2 (3)
C8—C9—H9B	109.4	C17—C22—H22	119.9
H9A—C9—H9B	108.0	C21—C22—H22	119.9
C10—N1—N2—N3	−0.2 (3)	N2—N1—C10—C11	−179.8 (3)
C9—N1—N2—N3	−173.8 (2)	C9—N1—C10—C11	−7.2 (4)
N1—N2—N3—C15	0.2 (3)	N1—C10—C11—C12	178.7 (3)
C6—C1—C2—C3	−0.6 (4)	C15—C10—C11—C12	−1.2 (4)
C1—C2—C3—F1	179.4 (3)	C10—C11—C12—C13	1.0 (5)
C1—C2—C3—C4	0.1 (5)	C11—C12—C13—C14	−0.5 (6)
F1—C3—C4—C5	−179.4 (3)	C12—C13—C14—C15	0.0 (5)
C2—C3—C4—C5	−0.1 (5)	N2—N3—C15—C10	−0.2 (3)
C3—C4—C5—C6	0.5 (4)	N2—N3—C15—C14	178.9 (3)
C4—C5—C6—C1	−0.9 (4)	N1—C10—C15—N3	0.1 (3)
C4—C5—C6—C7	−179.9 (2)	C11—C10—C15—N3	180.0 (2)
C2—C1—C6—C5	1.0 (4)	N1—C10—C15—C14	−179.1 (3)
C2—C1—C6—C7	180.0 (2)	C11—C10—C15—C14	0.8 (4)
C5—C6—C7—O1	177.5 (2)	C13—C14—C15—N3	−179.2 (3)
C1—C6—C7—O1	−1.5 (4)	C13—C14—C15—C10	−0.2 (5)
C5—C6—C7—C8	−2.0 (4)	C8—O2—C16—O3	−4.1 (3)
C1—C6—C7—C8	179.1 (2)	C8—O2—C16—C17	175.90 (19)
C16—O2—C8—C9	−175.00 (19)	O3—C16—C17—C22	0.6 (4)
C16—O2—C8—C7	64.7 (3)	O2—C16—C17—C22	−179.3 (2)
O1—C7—C8—O2	32.2 (3)	O3—C16—C17—C18	179.9 (3)
C6—C7—C8—O2	−148.3 (2)	O2—C16—C17—C18	−0.1 (3)
O1—C7—C8—C9	−85.2 (3)	C22—C17—C18—C19	−0.4 (4)
C6—C7—C8—C9	94.2 (3)	C16—C17—C18—C19	−179.6 (3)
N2—N1—C9—C8	83.0 (3)	C17—C18—C19—C20	−0.1 (5)
C10—N1—C9—C8	−89.1 (3)	C18—C19—C20—C21	0.6 (6)

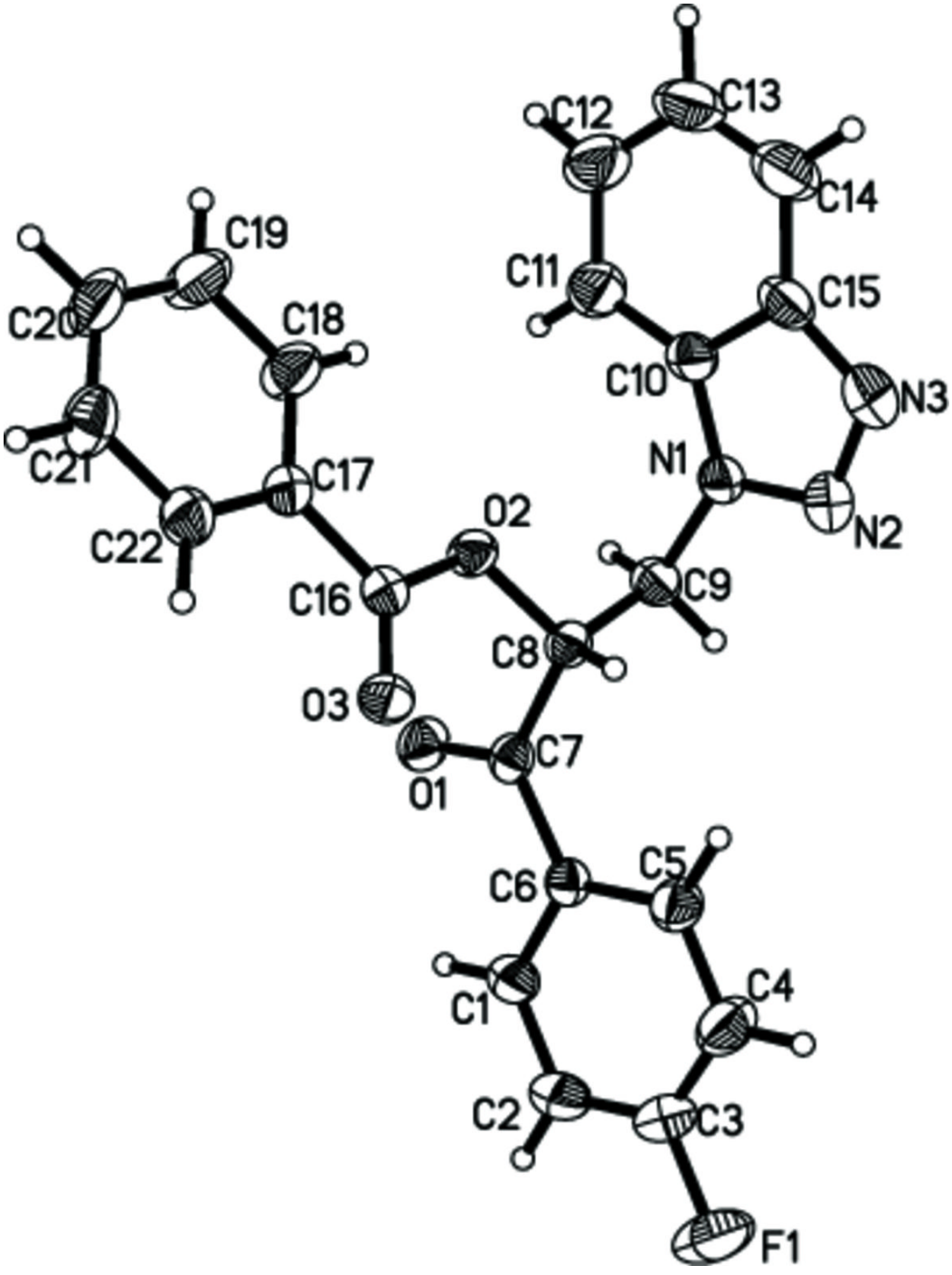
O2—C8—C9—N1	65.9 (2)	C19—C20—C21—C22	−0.6 (5)
C7—C8—C9—N1	−174.1 (2)	C18—C17—C22—C21	0.3 (4)
N2—N1—C10—C15	0.0 (3)	C16—C17—C22—C21	179.6 (2)
C9—N1—C10—C15	172.7 (2)	C20—C21—C22—C17	0.2 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.59	3.292 (5)	133
C8—H8···O1^{i}	0.98	2.50	3.470 (5)	173
C9—H9A···O3^{ii}	0.97	2.34	3.057 (4)	130
C1—H1···Cg^{ii}	0.93	2.95	3.730 (5)	143

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

Fig. 1


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