Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(1*H*-Benzotriazol-1-yl)-1-(4-fluorobenzoyl)ethyl isonicotinate

Jing Li,[a] Wu-Lan Zeng,[b] Ming-Hui Wang[a] 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

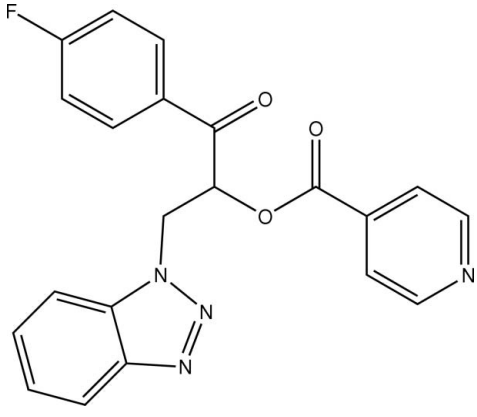
Received 29 August 2007; accepted 2 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.057; wR factor = 0.156; data-to-parameter ratio = 14.1.

Molecules of the title compound, $C_{21}H_{15}FN_4O_3$, are linked into chains along the b axis by intermolecular C—H···O hydrogen bonds. C—H···N interactions connect the chains into a three-dimensional network. The packing is further stabilized by C—H···π and π–π interactions [centroid–centroid distance 3.689 (2) Å].

Related literature

For a related structure, see: Han *et al.* (2007). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{15}FN_4O_3$
M_r = 390.37
Orthorhombic, *Pbca*
a = 18.475 (2) Å
b = 10.3014 (13) Å
c = 19.723 (3) Å
V = 3753.7 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.40 × 0.05 × 0.03 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.997
19822 measured reflections
3706 independent reflections
1930 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.156
S = 0.94
3706 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

*Cg*1 is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1^{i}	0.97	2.29	3.247 (4)	167
C12—H12A···N4^{ii}	0.93	2.48	3.386 (5)	164
C13—H13A···O3^{iii}	0.93	2.49	3.185 (5)	132
C15—H15B···O1^{i}	0.93	2.58	3.309 (4)	136
C1—H1A···Cg1^{iv}	0.93	3.08	3.811	137

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (iii) $x+\frac{1}{2}, y, -z+\frac{1}{2}$; (iv) $x, -y-\frac{3}{2}, z-\frac{1}{2}$.

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* and *PLATON* (Spek, 2003).

This project was supported by the Natural Science Foundation of Shandong Province (grants No. Z2006B01 and No. Y2006B07).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2347).

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.
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.

supplementary materials

Acta Cryst. (2007). E**63**, o4177 [**doi:10.1107/S1600536807042900**]

2-(1*H*-Benzotriazol-1-yl)-1-(4-fluorobenzoyl)ethyl isonicotinate

J. Li, W.-L. Zeng, M.-H. Wang and J. Wan

Comment

Recently we have 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 presented here.

All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable with those in the related compound, (II). The benzotriazole system is essentially planar, with a dihedral angle of 0.32 (2)/% between the triazole ring A (N1—N3/C10/C11) and benzene ring B (C10—C15). The mean plane of the benzotriazole group makes dihedral angles of 62.83 (1) and 51.71 (1)/% with the pyridine ring C (N4/C17—C21) and benzene ring D (C1—C6), respectively. The dihedral angle between the latter two aromatic C and D rings is 65.51 (2)/%.

In the crystal structure, molecules are linked into chains along the *b* axis by intermolecular C9—H9A···O1 and C15—H15B···O1 hydrogen bonds. C12—H12A···N4 interactions connect the chains into three-dimensional network (Fig. 2). The packing is further stabilized by a C—H···*Cg*1 (Table 1) interaction, *Cg*1 is the centroid of the C10···C15 ring. The distance of 3.689 /%A between the centroids of the triazole and pyridine rings with the symmetry code (1/2 − *x*, −1/2 + *y*, *z*) suggests a possible π-π interaction

Experimental

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

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic 0.98 Å, U_{iso} = 1.2U_{eq} (C) for CH, and 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2 atoms.

Figures

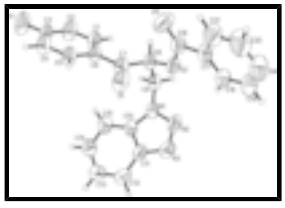


Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

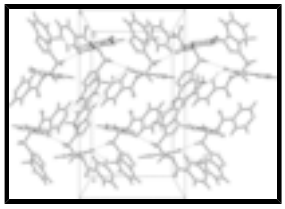


Fig. 2. A packing diagram of (I), viewed down the *c* axis. Hydrogen bonds are indicated by dashed lines.

2-(1*H*-Benzotriazol-1-yl)-1-(4-fluorobenzoyl)ethyl isonicotinate

Crystal data

$C_{21}H_{15}FN_4O_3$	F_{000} = 1616
M_r = 390.37	D_x = 1.382 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 1484 reflections
a = 18.475 (2) Å	θ = 2.3–18.3º
b = 10.3014 (13) Å	μ = 0.10 mm^{-1}
c = 19.723 (3) Å	*T* = 293 (2) K
V = 3753.7 (8) Å^3	Needle, colourless
Z = 8	0.40 × 0.05 × 0.03 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3706 independent reflections
Radiation source: fine-focus sealed tube	1930 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 2.1º
ω scans	*h* = −22→22
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*k* = −12→11
T_{min} = 0.960, T_{max} = 0.997	*l* = −24→19
19822 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
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H-atom parameters constrained
$wR(F^2)$ = 0.156	$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.9453P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.94	$(\Delta/\sigma)_{max} < 0.001$
3706 reflections	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
262 parameters	$\Delta\rho_{min}$ = −0.14 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}
O2	0.16082 (10)	0.45024 (19)	0.08610 (9)	0.0548 (5)
N1	0.30549 (13)	0.3692 (2)	0.11244 (11)	0.0514 (6)
C6	0.17406 (14)	0.3606 (3)	0.27131 (13)	0.0457 (7)
C8	0.17486 (15)	0.3570 (3)	0.13831 (12)	0.0496 (7)
H8A	0.1344	0.2959	0.1415	0.060*
O1	0.20182 (14)	0.5415 (2)	0.20452 (10)	0.0775 (7)
F1	0.14705 (13)	0.1940 (2)	0.45729 (9)	0.1040 (8)
N2	0.31636 (15)	0.4500 (3)	0.05856 (12)	0.0663 (7)
C7	0.18444 (16)	0.4281 (3)	0.20601 (13)	0.0509 (7)
C5	0.17641 (17)	0.4344 (3)	0.32980 (14)	0.0621 (8)
H5A	0.1847	0.5232	0.3265	0.074*
N3	0.37415 (16)	0.5183 (3)	0.06951 (14)	0.0735 (8)
C1	0.16128 (17)	0.2295 (3)	0.27654 (14)	0.0631 (9)
H1A	0.1582	0.1790	0.2376	0.076*
C9	0.24246 (16)	0.2864 (3)	0.11506 (13)	0.0533 (8)
H9A	0.2520	0.2148	0.1457	0.064*
H9B	0.2339	0.2503	0.0703	0.064*
C16	0.09670 (18)	0.5097 (3)	0.08663 (15)	0.0611 (8)
C4	0.16677 (17)	0.3796 (4)	0.39278 (15)	0.0691 (9)
H4A	0.1680	0.4298	0.4319	0.083*
O3	0.05007 (13)	0.4850 (3)	0.12680 (13)	0.0993 (9)
N4	0.0783 (2)	0.7918 (3)	−0.07079 (17)	0.0912 (10)
C10	0.35878 (15)	0.3866 (3)	0.15918 (14)	0.0507 (7)
C11	0.40250 (17)	0.4819 (3)	0.13141 (15)	0.0596 (8)
C17	0.09210 (16)	0.6081 (3)	0.03198 (14)	0.0571 (8)
C3	0.15539 (17)	0.2500 (4)	0.39558 (14)	0.0667 (9)
C18	0.14422 (17)	0.6214 (3)	−0.01731 (14)	0.0611 (8)
H18A	0.1853	0.5694	−0.0170	0.073*
C14	0.43413 (19)	0.3756 (4)	0.25411 (17)	0.0789 (11)
H14A	0.4464	0.3406	0.2960	0.095*
C2	0.1529 (2)	0.1726 (3)	0.33972 (16)	0.0749 (10)

H2B	0.1458	0.0836	0.3438	0.090*
C15	0.37350 (18)	0.3308 (3)	0.22210 (15)	0.0639 (9)
H15B	0.3440	0.2673	0.2410	0.077*
C19	0.1344 (2)	0.7133 (3)	−0.06715 (17)	0.0773 (10)
H19A	0.1698	0.7205	−0.1005	0.093*
C12	0.46429 (18)	0.5250 (4)	0.16520 (17)	0.0784 (10)
H12A	0.4945	0.5877	0.1465	0.094*
C13	0.47831 (18)	0.4714 (4)	0.22652 (18)	0.0844 (11)
H13A	0.5185	0.4994	0.2508	0.101*
C21	0.0339 (2)	0.6903 (4)	0.02977 (19)	0.0869 (12)
H21A	−0.0021	0.6859	0.0627	0.104*
C20	0.0296 (2)	0.7797 (4)	−0.0222 (2)	0.0998 (14)
H20A	−0.0102	0.8350	−0.0230	0.120*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0634 (13)	0.0589 (13)	0.0421 (11)	0.0086 (10)	0.0004 (9)	0.0122 (9)
N1	0.0660 (16)	0.0480 (15)	0.0402 (14)	0.0042 (12)	−0.0008 (12)	0.0070 (11)
C6	0.0536 (17)	0.0422 (18)	0.0414 (16)	0.0001 (13)	−0.0018 (12)	0.0060 (13)
C8	0.0675 (19)	0.0447 (17)	0.0368 (16)	−0.0024 (14)	−0.0034 (13)	0.0077 (13)
O1	0.137 (2)	0.0401 (13)	0.0549 (13)	−0.0157 (14)	0.0077 (13)	0.0036 (10)
F1	0.1483 (19)	0.1130 (18)	0.0508 (12)	−0.0085 (15)	0.0038 (12)	0.0284 (11)
N2	0.0780 (18)	0.075 (2)	0.0454 (15)	0.0038 (16)	0.0014 (13)	0.0197 (14)
C7	0.0677 (19)	0.0369 (18)	0.0483 (18)	0.0003 (15)	0.0013 (14)	0.0045 (13)
C5	0.091 (2)	0.0508 (19)	0.0440 (18)	−0.0044 (17)	−0.0018 (16)	−0.0043 (15)
N3	0.0739 (18)	0.083 (2)	0.0630 (18)	−0.0079 (17)	0.0051 (15)	0.0218 (15)
C1	0.098 (2)	0.050 (2)	0.0415 (17)	−0.0105 (17)	0.0004 (16)	0.0020 (14)
C9	0.073 (2)	0.0443 (18)	0.0424 (16)	0.0017 (15)	−0.0057 (14)	−0.0009 (13)
C16	0.062 (2)	0.071 (2)	0.0502 (19)	0.0072 (18)	−0.0022 (16)	0.0056 (16)
C4	0.090 (2)	0.073 (3)	0.0442 (19)	0.001 (2)	−0.0027 (16)	−0.0060 (17)
O3	0.0814 (16)	0.130 (2)	0.0862 (18)	0.0203 (16)	0.0256 (15)	0.0442 (16)
N4	0.110 (3)	0.086 (2)	0.077 (2)	0.019 (2)	−0.015 (2)	0.0247 (18)
C10	0.0622 (18)	0.0475 (18)	0.0425 (16)	0.0096 (15)	0.0003 (14)	0.0016 (13)
C11	0.0651 (19)	0.069 (2)	0.0453 (18)	−0.0006 (17)	0.0068 (16)	0.0102 (16)
C17	0.0650 (19)	0.061 (2)	0.0454 (17)	0.0086 (17)	−0.0085 (15)	0.0043 (15)
C3	0.082 (2)	0.083 (3)	0.0350 (18)	−0.001 (2)	0.0016 (15)	0.0171 (18)
C18	0.068 (2)	0.063 (2)	0.0514 (19)	0.0053 (17)	−0.0052 (16)	0.0065 (16)
C14	0.075 (2)	0.106 (3)	0.056 (2)	−0.002 (2)	−0.0099 (18)	0.017 (2)
C2	0.118 (3)	0.052 (2)	0.054 (2)	−0.013 (2)	0.0018 (19)	0.0131 (17)
C15	0.072 (2)	0.069 (2)	0.0512 (19)	−0.0052 (18)	−0.0030 (16)	0.0142 (16)
C19	0.097 (3)	0.075 (3)	0.060 (2)	0.005 (2)	−0.0071 (19)	0.0194 (19)
C12	0.068 (2)	0.101 (3)	0.066 (2)	−0.018 (2)	0.0084 (18)	0.013 (2)
C13	0.065 (2)	0.120 (3)	0.068 (2)	−0.018 (2)	−0.0033 (18)	0.006 (2)
C21	0.081 (3)	0.103 (3)	0.077 (3)	0.031 (2)	−0.0013 (19)	0.020 (2)
C20	0.101 (3)	0.104 (3)	0.095 (3)	0.047 (3)	−0.016 (3)	0.021 (3)

Geometric parameters (Å, °)

O2—C16	1.334 (3)	C4—H4A	0.9300
O2—C8	1.431 (3)	N4—C19	1.316 (4)
N1—C10	1.361 (3)	N4—C20	1.321 (5)
N1—N2	1.365 (3)	C10—C11	1.385 (4)
N1—C9	1.444 (4)	C10—C15	1.394 (4)
C6—C1	1.374 (4)	C11—C12	1.394 (4)
C6—C5	1.382 (4)	C17—C21	1.370 (4)
C6—C7	1.476 (4)	C17—C18	1.375 (4)
C8—C9	1.517 (4)	C3—C2	1.361 (4)
C8—C7	1.533 (4)	C18—C19	1.377 (4)
C8—H8A	0.9800	C18—H18A	0.9300
O1—C7	1.212 (3)	C14—C15	1.366 (4)
F1—C3	1.356 (3)	C14—C13	1.392 (5)
N2—N3	1.297 (3)	C14—H14A	0.9300
C5—C4	1.376 (4)	C2—H2B	0.9300
C5—H5A	0.9300	C15—H15B	0.9300
N3—C11	1.380 (4)	C19—H19A	0.9300
C1—C2	1.386 (4)	C12—C13	1.354 (4)
C1—H1A	0.9300	C12—H12A	0.9300
C9—H9A	0.9700	C13—H13A	0.9300
C9—H9B	0.9700	C21—C20	1.380 (5)
C16—O3	1.198 (3)	C21—H21A	0.9300
C16—C17	1.482 (4)	C20—H20A	0.9300
C4—C3	1.353 (5)		
C16—O2—C8	117.6 (2)	N1—C10—C15	133.6 (3)
C10—N1—N2	109.9 (2)	C11—C10—C15	122.0 (3)
C10—N1—C9	129.6 (2)	N3—C11—C10	108.7 (3)
N2—N1—C9	120.4 (2)	N3—C11—C12	130.3 (3)
C1—C6—C5	118.9 (3)	C10—C11—C12	120.9 (3)
C1—C6—C7	123.4 (3)	C21—C17—C18	117.7 (3)
C5—C6—C7	117.7 (3)	C21—C17—C16	119.4 (3)
O2—C8—C9	104.7 (2)	C18—C17—C16	122.9 (3)
O2—C8—C7	109.1 (2)	C4—C3—F1	118.3 (3)
C9—C8—C7	113.4 (2)	C4—C3—C2	123.4 (3)
O2—C8—H8A	109.8	F1—C3—C2	118.3 (3)
C9—C8—H8A	109.8	C17—C18—C19	118.8 (3)
C7—C8—H8A	109.8	C17—C18—H18A	120.6
N3—N2—N1	108.8 (2)	C19—C18—H18A	120.6
O1—C7—C6	120.6 (3)	C15—C14—C13	122.7 (3)
O1—C7—C8	118.0 (2)	C15—C14—H14A	118.7
C6—C7—C8	121.3 (2)	C13—C14—H14A	118.7
C4—C5—C6	121.6 (3)	C3—C2—C1	118.4 (3)
C4—C5—H5A	119.2	C3—C2—H2B	120.8
C6—C5—H5A	119.2	C1—C2—H2B	120.8
N2—N3—C11	108.2 (2)	C14—C15—C10	115.6 (3)
C6—C1—C2	120.2 (3)	C14—C15—H15B	122.2

C6—C1—H1A	119.9	C10—C15—H15B	122.2
C2—C1—H1A	119.9	N4—C19—C18	124.4 (4)
N1—C9—C8	113.0 (2)	N4—C19—H19A	117.8
N1—C9—H9A	109.0	C18—C19—H19A	117.8
C8—C9—H9A	109.0	C13—C12—C11	117.0 (3)
N1—C9—H9B	109.0	C13—C12—H12A	121.5
C8—C9—H9B	109.0	C11—C12—H12A	121.5
H9A—C9—H9B	107.8	C12—C13—C14	121.7 (3)
O3—C16—O2	123.1 (3)	C12—C13—H13A	119.1
O3—C16—C17	125.8 (3)	C14—C13—H13A	119.1
O2—C16—C17	111.1 (3)	C17—C21—C20	118.8 (4)
C3—C4—C5	117.5 (3)	C17—C21—H21A	120.6
C3—C4—H4A	121.3	C20—C21—H21A	120.6
C5—C4—H4A	121.3	N4—C20—C21	124.2 (4)
C19—N4—C20	116.1 (3)	N4—C20—H20A	117.9
N1—C10—C11	104.3 (2)	C21—C20—H20A	117.9
C16—O2—C8—C9	167.5 (2)	N2—N3—C11—C12	179.0 (3)
C16—O2—C8—C7	−70.8 (3)	N1—C10—C11—N3	0.0 (3)
C10—N1—N2—N3	−0.3 (3)	C15—C10—C11—N3	−179.7 (3)
C9—N1—N2—N3	176.9 (2)	N1—C10—C11—C12	−179.3 (3)
C1—C6—C7—O1	−173.5 (3)	C15—C10—C11—C12	1.0 (5)
C5—C6—C7—O1	7.5 (4)	O3—C16—C17—C21	7.9 (5)
C1—C6—C7—C8	5.5 (4)	O2—C16—C17—C21	−171.9 (3)
C5—C6—C7—C8	−173.5 (3)	O3—C16—C17—C18	−172.3 (3)
O2—C8—C7—O1	−22.7 (4)	O2—C16—C17—C18	7.9 (4)
C9—C8—C7—O1	93.6 (3)	C5—C4—C3—F1	178.9 (3)
O2—C8—C7—C6	158.3 (2)	C5—C4—C3—C2	−0.1 (5)
C9—C8—C7—C6	−85.5 (3)	C21—C17—C18—C19	−1.9 (5)
C1—C6—C5—C4	0.4 (5)	C16—C17—C18—C19	178.3 (3)
C7—C6—C5—C4	179.5 (3)	C4—C3—C2—C1	−1.1 (5)
N1—N2—N3—C11	0.4 (3)	F1—C3—C2—C1	179.9 (3)
C5—C6—C1—C2	−1.7 (5)	C6—C1—C2—C3	2.1 (5)
C7—C6—C1—C2	179.2 (3)	C13—C14—C15—C10	0.6 (5)
C10—N1—C9—C8	96.4 (3)	N1—C10—C15—C14	179.8 (3)
N2—N1—C9—C8	−80.3 (3)	C11—C10—C15—C14	−0.6 (5)
O2—C8—C9—N1	65.1 (3)	C20—N4—C19—C18	0.7 (6)
C7—C8—C9—N1	−53.7 (3)	C17—C18—C19—N4	0.8 (5)
C8—O2—C16—O3	−3.0 (5)	N3—C11—C12—C13	179.5 (3)
C8—O2—C16—C17	176.8 (2)	C10—C11—C12—C13	−1.4 (5)
C6—C5—C4—C3	0.5 (5)	C11—C12—C13—C14	1.4 (6)
N2—N1—C10—C11	0.2 (3)	C15—C14—C13—C12	−1.1 (6)
C9—N1—C10—C11	−176.7 (3)	C18—C17—C21—C20	1.4 (5)
N2—N1—C10—C15	179.9 (3)	C16—C17—C21—C20	−178.7 (3)
C9—N1—C10—C15	3.0 (5)	C19—N4—C20—C21	−1.2 (6)
N2—N3—C11—C10	−0.3 (4)	C17—C21—C20—N4	0.1 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C9—H9A···O1^{i}	0.97	2.29	3.247 (4)	167
C12—H12A···N4^{ii}	0.93	2.48	3.386 (5)	164
C13—H13A···O3^{iii}	0.93	2.49	3.185 (5)	132
C15—H15B···O1^{i}	0.93	2.58	3.309 (4)	136
C1—H1A···Cg1^{iv}	0.93	3.08	3.811	137

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*; (ii) *x*+1/2, −*y*+3/2, −*z*; (iii) *x*+1/2, *y*, −*z*+1/2; (iv) *x*, −*y*−3/2, *z*−1/2.

Fig. 1

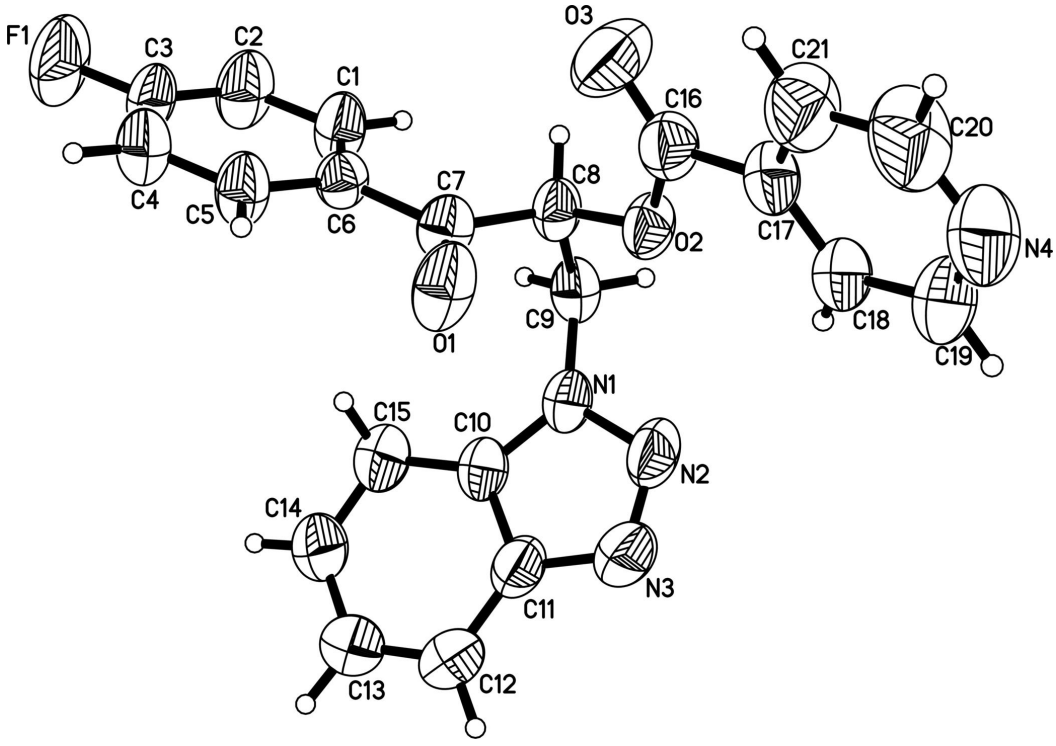

F1
C3
C2
C1
O3
C16
C21
C20
C4
C5
C6
C7
C8
O2
C17
N4
O1
C9
C18
C19
N1
C15
C10
N2
C14
N3
C11
C13
C12

Fig. 2