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(*Z*)-Ethyl 3-benzamido-2-cyano-3-(4-fluorophenyl)acrylate

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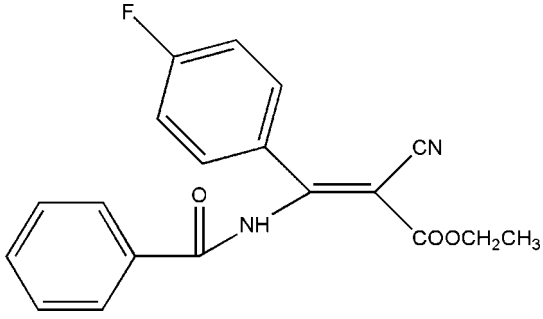
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.057; wR factor = 0.124; data-to-parameter ratio = 8.4.

The title compound, $C_{19}H_{15}FN_2O_3$, was prepared by the reaction of (*Z*)-ethyl 3-amino-2-cyano-3-(4-fluorophenyl)-acrylate and benzoyl chloride. In addition to an intramolecular N—H···O hydrogen bond, the crystal packing shows the molecules to be connected by intermolecular C—H···O and C—H···N hydrogen bonds. The ethyl group is disordered over two positions, with site-occupancy factors of 0.75 and 0.25.

Related literature

Several acrylate compounds are useful as inhibitors of *Pyricularia oryzae*, *Rhizoctonia solani*, *Botrytis cinerea* and *Gibberella zeae* (Heller *et al.*, 2004; Creagh & Hubbell, 1992; Ibers & Hamilton, 1964).



Experimental

Crystal data

$C_{19}H_{15}FN_2O_3$
M_r = 338.33
Orthorhombic, $P2_12_12_1$
a = 6.2149 (5) Å
b = 14.138 (1) Å
c = 19.050 (1) Å
V = 1673.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 292 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: none
15612 measured reflections
2109 independent reflections
1634 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.124
S = 1.11
2109 reflections
250 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.89 (4)	1.86 (4)	2.653 (4)	146 (3)
C14—H14···O1^{i}	0.93	2.56	3.202 (5)	126
C5—H5···N2^{ii}	0.93	2.50	3.413 (5)	167

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2031).

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supplementary materials

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(*Z*)-Ethyl 3-benzamido-2-cyano-3-(4-fluorophenyl)acrylate

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Comment

The title compound is useful as an inhibitor of Pyricularia oryzae, Rhizoctonia solani, Botrytis cinerea and Gibberella zeae (Heller *et al.* 2004; Creagh & Hubbell, 1992; Ibers & Hamilton, 1964). Recently, we obtained single crystals of this compound, and its crystal structure is reported here. The molecular conformation is stabilized by intramolecular C—H···O and N—H···O hydrogen bonds (Table 1). The crystal packing is governed by additional C—H···N and C—H···O interactions.

Experimental

To a solution of (*Z*)-ethyl 3-amino-2-cyano-3-(4-fluorophenyl)acrylate (1.17 g,0.0050 mol) in CH_2Cl_2 (18 ml), benzoyl chloride (2.11 g,0.015 mol) was added. Subsequently, Et_3N (1.52 g,0.015 mol) was dropped into the solution under stirring. The reaction mixture was then heated to reflux and stirred for 4 h. Subsequently, it was cooled to room temperature, the reaction solution was filtered off and some white solid was separated. The organic phase was washed with water and then dried over Na_2SO_4. After removal of the solvent, a brown dope was obtained. After column chromatography using ethyl acetate/light petroleum (1:6) as the eluent, the pure E-isomer is separated from the mother liquid as colorless prismatic crystals. Small single crystals were grown from a solution of ethyl acetate/light petroleum (3:1) after 45 days, at room temperature.

Refinement

The position of H1 was determined from the difference Fourier map and was refined without constraints. Methyl H atoms were placed in calculated positions with C—H=0.96 Å and the torsion angle was refined to fit the electron density; thermal parameters were refined as U_{iso}(H)=1.5U_{eq}(C). Other H atoms were placed in calculated positions with C—H = 0.96 Å (methylene) and 0.93 Å (aromatic C—H), and refined using a riding model, with U_{iso}(H)=1.2U_{eq}(C). In the absence of significant anomalous scattering, Friedel pairs were merged.

Figures

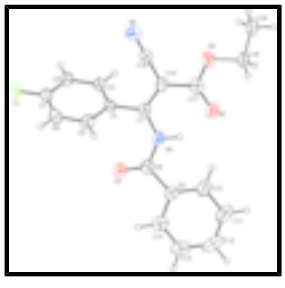

Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 30% propability level and the atom-numbering scheme.

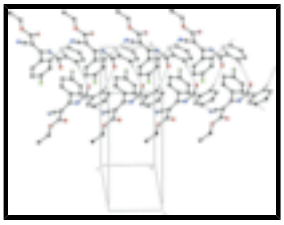

Fig. 2. The packing of (I), viewed down the *c* axis showing one layer of molecules connected by intermolecular C(14)—H(14)···O(1) and C(5)—H(5)···N(2) hydrogen bonds.

(*Z*)-ethyl 3-(benzamido)-2-cyano-3-(4-fluorophenyl)acrylate

Crystal data

$C_{19}H_{15}FN_2O_3$	F_{000} = 704
M_r = 338.33	D_x = 1.343 Mg m^{-3}
Orthorhombic, *P*2(1)2(1)2(1)	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P2ac2ab	Cell parameters from 2229 reflections
a = 6.2149 (5) Å	θ = 2.6–21.4º
b = 14.138 (1) Å	μ = 0.10 mm^{-1}
c = 19.050 (1) Å	*T* = 292 (2) K
V = 1673.8 (2) Å^3	Needle, colorless
Z = 4	0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1634 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.052
Monochromator: graphite	θ_{max} = 27.0º
T = 292(2) K	θ_{min} = 1.8º
phi and ω scans	*h* = −7→7
Absorption correction: none	*k* = −14→18
15612 measured reflections	*l* = −24→24
2109 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.057	$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.3759P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.124	$(\Delta/\sigma)_{max} < 0.001$
S = 1.11	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
2109 reflections	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
250 parameters	Extinction correction: none
4 restraints	Absolute structure: Flack (1983)

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Flack parameter: 0 (10)

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}	Occ. (<1)
C1	0.5735 (7)	0.8275 (3)	0.24083 (18)	0.0574 (10)	
C2	0.7450 (7)	0.8137 (2)	0.19792 (18)	0.0548 (9)	
H2	0.8569	0.8574	0.1961	0.066*	
C3	0.7488 (6)	0.7328 (2)	0.15683 (17)	0.0480 (8)	
H3	0.8650	0.7216	0.1272	0.058*	
C4	0.5810 (5)	0.6683 (2)	0.15954 (14)	0.0412 (7)	
C5	0.4083 (6)	0.6857 (3)	0.20415 (17)	0.0587 (10)	
H5	0.2945	0.6431	0.2062	0.070*	
C6	0.4053 (7)	0.7653 (3)	0.24518 (19)	0.0664 (11)	
H6	0.2909	0.7768	0.2755	0.080*	
C7	0.5925 (6)	0.5794 (2)	0.11847 (15)	0.0433 (8)	
C8	0.2774 (6)	0.6138 (3)	0.04035 (17)	0.0533 (9)	
C9	0.1542 (6)	0.5683 (3)	−0.01794 (16)	0.0508 (9)	
C10	0.2301 (8)	0.4928 (3)	−0.05696 (19)	0.0707 (11)	
H10	0.3628	0.4659	−0.0464	0.085*	
C11	0.1081 (9)	0.4574 (3)	−0.1117 (2)	0.0879 (15)	
H11	0.1609	0.4077	−0.1387	0.106*	
C12	−0.0893 (9)	0.4948 (4)	−0.1265 (2)	0.0926 (18)	
H12	−0.1738	0.4691	−0.1620	0.111*	
C13	−0.1612 (8)	0.5702 (4)	−0.0887 (2)	0.0806 (14)	
H13	−0.2938	0.5969	−0.0997	0.097*	
C14	−0.0433 (6)	0.6077 (3)	−0.03491 (19)	0.0640 (11)	
H14	−0.0952	0.6594	−0.0099	0.077*	
C15	0.7524 (6)	0.5153 (2)	0.13150 (15)	0.0459 (8)	
C16	0.8881 (6)	0.5289 (2)	0.19117 (18)	0.0472 (8)	
C17	0.7806 (7)	0.4278 (3)	0.09120 (18)	0.0570 (10)	
C18	0.976 (2)	0.2890 (7)	0.0723 (5)	0.072 (3)	0.75 (2)
H18A	1.0026	0.3004	0.0228	0.087*	0.75 (2)
H18B	0.8489	0.2499	0.0770	0.087*	0.75 (2)
C19	1.1684 (18)	0.2416 (9)	0.1059 (6)	0.087 (4)	0.75 (2)

H19A	1.2945	0.2795	0.0984	0.131*	0.75 (2)
H19B	1.1893	0.1803	0.0853	0.131*	0.75 (2)
H19C	1.1435	0.2348	0.1554	0.131*	0.75 (2)
C18'	1.081 (6)	0.3096 (18)	0.0732 (17)	0.084 (10)	0.25 (2)
H18C	1.2306	0.3285	0.0735	0.101*	0.25 (2)
H18D	1.0332	0.3045	0.0248	0.101*	0.25 (2)
C19'	1.053 (9)	0.214 (2)	0.111 (2)	0.131 (14)	0.25 (2)
H19D	1.1194	0.2175	0.1565	0.196*	0.25 (2)
H19E	1.1203	0.1652	0.0839	0.196*	0.25 (2)
H19F	0.9027	0.2005	0.1162	0.196*	0.25 (2)
F1	0.5689 (5)	0.90628 (18)	0.28136 (12)	0.0907 (9)	
N1	0.4415 (5)	0.5588 (2)	0.06813 (15)	0.0554 (8)	
H1	0.471 (6)	0.503 (3)	0.0484 (19)	0.066*	
N2	0.9903 (6)	0.5370 (2)	0.24060 (17)	0.0661 (9)	
O1	0.2334 (5)	0.69149 (19)	0.06227 (14)	0.0737 (8)	
O2	0.6578 (5)	0.39995 (18)	0.04527 (14)	0.0725 (8)	
O3	0.9497 (5)	0.3796 (2)	0.11071 (14)	0.0772 (9)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.068 (3)	0.051 (2)	0.0531 (18)	0.012 (2)	0.000 (2)	−0.0122 (17)
C2	0.061 (2)	0.0410 (19)	0.062 (2)	−0.004 (2)	−0.004 (2)	−0.0069 (17)
C3	0.0492 (19)	0.0437 (19)	0.0510 (17)	−0.0010 (19)	0.0071 (17)	−0.0026 (15)
C4	0.0406 (18)	0.0435 (18)	0.0396 (14)	0.0007 (17)	0.0026 (15)	0.0003 (13)
C5	0.049 (2)	0.067 (3)	0.0600 (19)	−0.014 (2)	0.0106 (18)	−0.0049 (19)
C6	0.054 (2)	0.086 (3)	0.059 (2)	0.007 (3)	0.017 (2)	−0.017 (2)
C7	0.0448 (18)	0.0430 (18)	0.0423 (15)	−0.0059 (17)	0.0085 (15)	0.0009 (14)
C8	0.056 (2)	0.051 (2)	0.0532 (18)	−0.004 (2)	0.0010 (18)	0.0007 (17)
C9	0.055 (2)	0.054 (2)	0.0434 (16)	−0.0096 (19)	−0.0018 (16)	0.0066 (16)
C10	0.090 (3)	0.060 (2)	0.063 (2)	−0.003 (3)	−0.013 (2)	−0.0096 (19)
C11	0.121 (4)	0.076 (3)	0.067 (2)	−0.016 (3)	−0.027 (3)	−0.006 (2)
C12	0.104 (4)	0.106 (4)	0.068 (3)	−0.052 (4)	−0.037 (3)	0.018 (3)
C13	0.063 (3)	0.108 (4)	0.071 (3)	−0.019 (3)	−0.018 (2)	0.025 (3)
C14	0.059 (3)	0.077 (3)	0.0555 (19)	−0.009 (2)	−0.001 (2)	0.014 (2)
C15	0.0551 (19)	0.0372 (18)	0.0452 (16)	−0.0031 (19)	0.0041 (16)	0.0007 (14)
C16	0.046 (2)	0.0417 (19)	0.0542 (18)	−0.0002 (17)	0.0063 (17)	0.0043 (16)
C17	0.078 (3)	0.044 (2)	0.0492 (18)	0.002 (2)	0.006 (2)	0.0063 (17)
C18	0.086 (6)	0.060 (5)	0.071 (4)	0.021 (5)	−0.019 (5)	−0.027 (3)
C19	0.113 (7)	0.065 (6)	0.083 (5)	0.032 (5)	−0.023 (6)	−0.024 (5)
C18'	0.065 (17)	0.10 (2)	0.086 (14)	0.031 (17)	−0.020 (17)	−0.039 (16)
C19'	0.13 (4)	0.13 (3)	0.13 (2)	−0.02 (3)	0.00 (3)	−0.01 (2)
F1	0.104 (2)	0.0759 (17)	0.0920 (16)	0.0136 (17)	0.0071 (16)	−0.0396 (13)
N1	0.065 (2)	0.0439 (17)	0.0577 (16)	0.0022 (17)	−0.0118 (16)	−0.0106 (14)
N2	0.062 (2)	0.071 (2)	0.0657 (18)	−0.001 (2)	−0.0089 (17)	0.0033 (17)
O1	0.0789 (19)	0.0590 (17)	0.0833 (17)	0.0130 (17)	−0.0195 (17)	−0.0171 (15)
O2	0.096 (2)	0.0507 (16)	0.0705 (16)	0.0077 (16)	−0.0151 (17)	−0.0137 (13)
O3	0.098 (2)	0.0618 (17)	0.0722 (16)	0.0301 (18)	−0.0121 (17)	−0.0125 (14)

Geometric parameters (Å, °)

C1—F1	1.355 (4)	C12—H12	0.9300
C1—C2	1.358 (5)	C13—C14	1.367 (6)
C1—C6	1.369 (6)	C13—H13	0.9300
C2—C3	1.387 (4)	C14—H14	0.9300
C2—H2	0.9300	C15—C16	1.428 (5)
C3—C4	1.386 (5)	C15—C17	1.466 (5)
C3—H3	0.9300	C16—N2	1.142 (4)
C4—C5	1.391 (5)	C17—O2	1.226 (4)
C4—C7	1.483 (4)	C17—O3	1.306 (5)
C5—C6	1.370 (5)	C18—O3	1.486 (6)
C5—H5	0.9300	C18—C19	1.511 (8)
C6—H6	0.9300	C18—H18A	0.9700
C7—C15	1.368 (5)	C18—H18B	0.9700
C7—N1	1.373 (4)	C19—H19A	0.9600
C8—O1	1.207 (4)	C19—H19B	0.9600
C8—N1	1.388 (5)	C19—H19C	0.9600
C8—C9	1.494 (5)	C18'—O3	1.467 (10)
C9—C10	1.384 (5)	C18'—C19'	1.538 (11)
C9—C14	1.386 (5)	C18'—H18C	0.9700
C10—C11	1.384 (6)	C18'—H18D	0.9700
C10—H10	0.9300	C19'—H19D	0.9600
C11—C12	1.365 (7)	C19'—H19E	0.9600
C11—H11	0.9300	C19'—H19F	0.9600
C12—C13	1.362 (7)	N1—H1	0.89 (4)
F1—C1—C2	118.5 (4)	C12—C13—C14	121.6 (5)
F1—C1—C6	118.5 (3)	C12—C13—H13	119.2
C2—C1—C6	122.9 (3)	C14—C13—H13	119.2
C1—C2—C3	118.2 (4)	C13—C14—C9	119.5 (4)
C1—C2—H2	120.9	C13—C14—H14	120.2
C3—C2—H2	120.9	C9—C14—H14	120.2
C4—C3—C2	120.6 (3)	C7—C15—C16	118.9 (3)
C4—C3—H3	119.7	C7—C15—C17	123.4 (3)
C2—C3—H3	119.7	C16—C15—C17	117.4 (3)
C3—C4—C5	119.2 (3)	N2—C16—C15	176.8 (4)
C3—C4—C7	120.1 (3)	O2—C17—O3	122.5 (4)
C5—C4—C7	120.6 (3)	O2—C17—C15	124.8 (4)
C6—C5—C4	120.3 (4)	O3—C17—C15	112.7 (4)
C6—C5—H5	119.9	O3—C18—C19	105.2 (7)
C4—C5—H5	119.9	O3—C18—H18A	110.7
C1—C6—C5	118.9 (3)	C19—C18—H18A	110.7
C1—C6—H6	120.6	O3—C18—H18B	110.7
C5—C6—H6	120.6	C19—C18—H18B	110.7
C15—C7—N1	118.9 (3)	H18A—C18—H18B	108.8
C15—C7—C4	120.1 (3)	O3—C18'—C19'	108 (3)
N1—C7—C4	121.1 (3)	O3—C18'—H18C	110.2
O1—C8—N1	123.0 (3)	C19'—C18'—H18C	110.2

O1—C8—C9	122.2 (4)	O3—C18'—H18D	110.2
N1—C8—C9	114.8 (3)	C19'—C18'—H18D	110.2
C10—C9—C14	119.2 (4)	H18C—C18'—H18D	108.5
C10—C9—C8	123.8 (4)	C18'—C19'—H19D	109.5
C14—C9—C8	117.0 (4)	C18'—C19'—H19E	109.5
C11—C10—C9	119.8 (4)	H19D—C19'—H19E	109.5
C11—C10—H10	120.1	C18'—C19'—H19F	109.5
C9—C10—H10	120.1	H19D—C19'—H19F	109.5
C12—C11—C10	120.5 (5)	H19E—C19'—H19F	109.5
C12—C11—H11	119.8	C7—N1—C8	130.5 (3)
C10—C11—H11	119.8	C7—N1—H1	110 (2)
C13—C12—C11	119.3 (4)	C8—N1—H1	119 (2)
C13—C12—H12	120.3	C17—O3—C18'	131.2 (16)
C11—C12—H12	120.3	C17—O3—C18	113.5 (4)
F1—C1—C2—C3	179.7 (3)	C10—C9—C14—C13	1.4 (5)
C6—C1—C2—C3	0.0 (6)	C8—C9—C14—C13	178.7 (3)
C1—C2—C3—C4	0.3 (5)	N1—C7—C15—C16	−169.8 (3)
C2—C3—C4—C5	−0.1 (5)	C4—C7—C15—C16	8.7 (4)
C2—C3—C4—C7	−176.5 (3)	N1—C7—C15—C17	4.2 (5)
C3—C4—C5—C6	−0.4 (5)	C4—C7—C15—C17	−177.2 (3)
C7—C4—C5—C6	176.0 (3)	C7—C15—C16—N2	94 (7)
F1—C1—C6—C5	179.7 (4)	C17—C15—C16—N2	−80 (7)
C2—C1—C6—C5	−0.5 (6)	C7—C15—C17—O2	−4.9 (6)
C4—C5—C6—C1	0.7 (6)	C16—C15—C17—O2	169.2 (3)
C3—C4—C7—C15	61.6 (4)	C7—C15—C17—O3	176.9 (3)
C5—C4—C7—C15	−114.7 (4)	C16—C15—C17—O3	−8.9 (5)
C3—C4—C7—N1	−119.9 (4)	C15—C7—N1—C8	−173.3 (3)
C5—C4—C7—N1	63.8 (4)	C4—C7—N1—C8	8.2 (5)
O1—C8—C9—C10	162.1 (4)	O1—C8—N1—C7	−5.7 (6)
N1—C8—C9—C10	−19.5 (5)	C9—C8—N1—C7	175.9 (3)
O1—C8—C9—C14	−15.1 (5)	O2—C17—O3—C18'	25.4 (19)
N1—C8—C9—C14	163.3 (3)	C15—C17—O3—C18'	−156.4 (19)
C14—C9—C10—C11	−0.5 (6)	O2—C17—O3—C18	−0.3 (8)
C8—C9—C10—C11	−177.6 (4)	C15—C17—O3—C18	177.9 (7)
C9—C10—C11—C12	−1.7 (7)	C19'—C18'—O3—C17	−115 (4)
C10—C11—C12—C13	2.8 (7)	C19'—C18'—O3—C18	−56 (4)
C11—C12—C13—C14	−1.9 (7)	C19—C18—O3—C17	−175.9 (11)
C12—C13—C14—C9	−0.2 (6)	C19—C18—O3—C18'	48 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.89 (4)	1.86 (4)	2.653 (4)	146 (3)
C14—H14···O1^{i}	0.93	2.56	3.202 (5)	126
C5—H5···N2^{ii}	0.93	2.50	3.413 (5)	167

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

Fig. 1

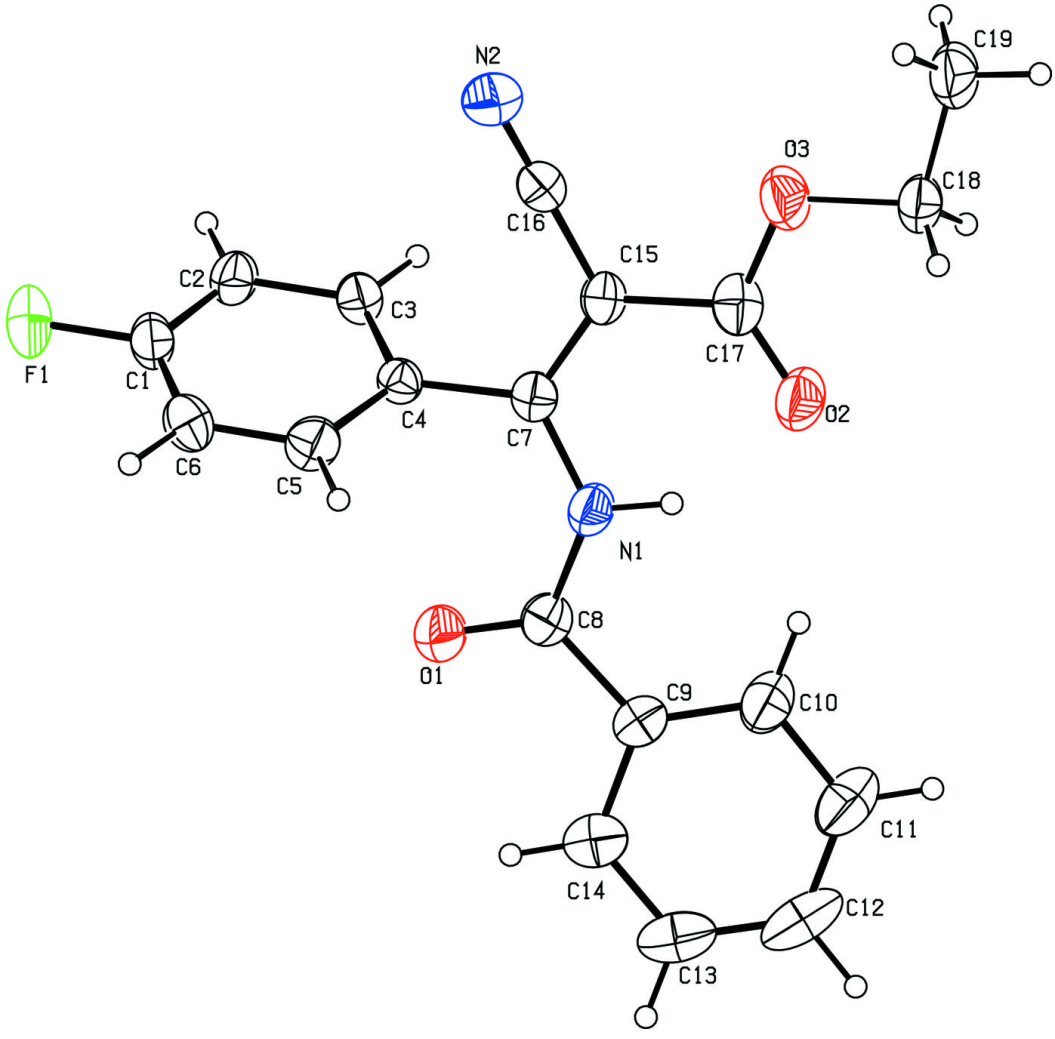
N2
C19
O3
C18
C16
C15
C2
C3
C17
F1
C1
C4
C7
O2
C6
C5
N1
C8
O1
C9
C10
C11
C14
C12
C13

Fig. 2