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(Z)-Ethyl 3-(4-chloro-3-ethyl-1-methyl-1*H*-pyrazole-5-carboxamido)-2-cyano-3-(4-fluorophenyl)acrylate

Dehua Zhang,[a]* Xiaoyan Zhang[b] and Yang Liu[c]

[a]Department of Chemistry and Environmental Engineering, Hubei Normal University, Huangshi 435002, People's Republic of China, [b]School of Mathematics and Physics, Huangshi Institute of Technology, Huangshi 435003, People's Republic of China, and [c]Key Laboratory of Pesticides and Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, 152 Luoyu Road, Wuhan 430079, People's Republic of China
Correspondence e-mail: zhangdehua200@163.com

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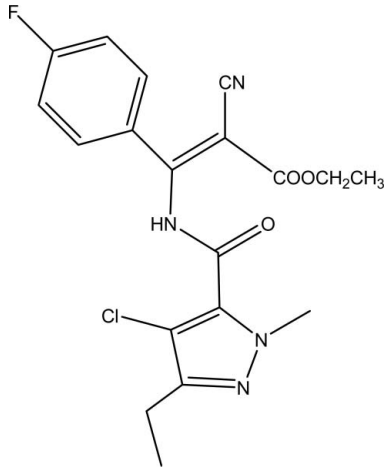
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.061; wR factor = 0.145; data-to-parameter ratio = 15.0.

The title compound, $C_{19}H_{18}ClFN_4O_3$, was prepared by the reaction of (Z)-ethyl 3-amino-2-cyano-3-(4-fluorophenyl)-acrylate and 4-chloro-3-ethyl-1-methyl-1*H*-pyrazole-5-carbonyl chloride. The planar pyrazole ring is perpendicular to the benzene ring [dihedral angle 89.70 (10)°]. The molecular conformation is stabilized by intramolecular C—H···O, N—H···O and N—H···Cl hydrogen bonds.

Related literature

For related literature, see: Heller *et al.* (2004).



Experimental

Crystal data

$C_{19}H_{18}ClFN_4O_3$
M_r = 404.82
Monoclinic, $P2_1/c$
a = 8.7594 (7) Å
b = 28.192 (3) Å
c = 8.5160 (8) Å
β = 109.885 (2)°
V = 1977.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 294 (2) K
0.20 × 0.10 × 0.04 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: none
20334 measured reflections
3888 independent reflections
1860 reflections with $I > 2\sigma(I)$
R_{int} = 0.123

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.145
S = 0.91
3888 reflections
259 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19B···O3	0.96	2.31	2.983 (4)	126
N2—H2A···O1	0.87 (3)	1.93 (3)	2.653 (3)	139 (3)
N2—H2A···Cl1	0.87 (3)	2.70 (3)	3.110 (3)	110 (3)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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, 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: RZ2156).

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supplementary materials

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(Z)-Ethyl 3-(4-chloro-3-ethyl-1-methyl-1*H*-pyrazole-5-carboxamido)-2-cyano-3-(4-fluorophenyl)acrylate

D. Zhang, X. Zhang and Y. Liu

Comment

The title compound is useful as an inhibitor of Pyricularia oryzae, Rhizoctonia solani, Botrytis cinerea and Gibberella zeae. Recently we obtained single crystals of this compound (Heller *et al.*, 2004), and its crystal structure is reported here.

In the molecule of the title compound (Fig. 1), all bond lengths and angles are unexceptional. The pyrazole ring is planar (maximum deviation 0.007 (3) Å for atoms C14 and C15) and oriented perpendicular to the benzene ring, the dihedral angle they form being 89.70 (10)°. The molecular conformation is stabilized by intramolecular C—H···O, N—H···O and N—H···Cl hydrogen bonds (Table 1). The crystal packing is governed only by van der Waals interactions.

Experimental

To a solution of (*Z*)-ethyl 3-amino-2-cyano-3-(4-fluorophenyl)acrylate (1.17 g, 5 mmol) in CH_2Cl_2 (18 ml), 4-chloro-3-ethyl-1-methyl-1*H*-pyrazole-5-carbonyl chloride (3.88 g, 15 mmol) was added. Subsequently, Et_3N (1.52 g, 15 mmol) was dropped into the solution under stirring and the reaction mixture was heated to reflux and stirred for 4 h. After cooling to room temperature, the mixture was filtered off and the resulting white solid was separated. The organic phase was washed with water and dried over anhydrous Na_2SO_4. After removal of the solvent, a brown dope was obtained. Pure E-isomer of the title compound was separated from the mother liquid by column chromatography. Single crystal suitable for X-ray analysis were obtain by slow evaporation of an ethyl acetate/petroleum ether (3:1 *v*/*v*) solution at room temperature over a period of 45 days.

Refinement

The amino H atom was located in a difference Fourier map and refined with a distance restraint [N—H = 0.87 (3) Å]. 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, with U_{iso}(H) = 1.5 U_{eq}(C). Other H atoms were placed in calculated positions with C—H = 0.93–0.97 Å and refined in the riding mode with U_{iso}(H) = 1.2U_{eq}(C). The ration of observed/unique reflections is low (48%), and the value of R_{int} is 0.12, due to the poor quality of the diffraction.

Figures

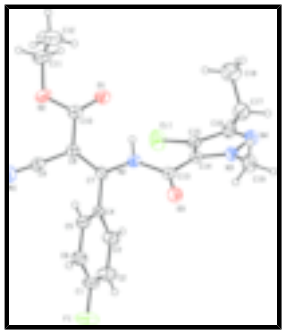


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

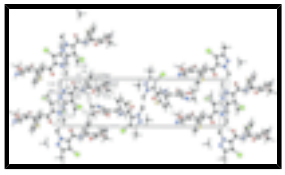


Fig. 2. Packing diagram of the title compound, viewed down the *a* axis.

(*Z*)-Ethyl 3-(4-chloro-3-ethyl-1-methyl-1*H*-pyrazole-5-carboxamido)- 2-cyano-3-(4-fluorophenyl)acrylate

Crystal data

$C_{19}H_{18}ClFN_4O_3$	F_{000} = 840
M_r = 404.82	D_x = 1.360 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1853 reflections
a = 8.7594 (7) Å	θ = 2.5–19.4º
b = 28.192 (3) Å	μ = 0.23 mm^{-1}
c = 8.5160 (8) Å	T = 294 (2) K
β = 109.885 (2)º	Plate, colourless
V = 1977.6 (3) Å^3	0.20 × 0.10 × 0.04 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1860 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.123
Monochromator: graphite	θ_{max} = 26.0º
T = 294(2) K	θ_{min} = 1.4º
φ and ω scans	h = −10→10
Absorption correction: none	k = −34→34
20334 measured reflections	l = −10→9
3888 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.061$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.145$	$w = 1/[\sigma^2(F_o^2) + (0.058P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.91$	$(\Delta/\sigma)_{max} < 0.001$
3888 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
259 parameters	$\Delta\rho_{min} = -0.33$ 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 $F^2 > 2$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}
C1	0.0303 (4)	0.12352 (12)	0.9437 (5)	0.0510 (9)
C2	0.0405 (4)	0.10853 (13)	0.7953 (5)	0.0628 (11)
H2	−0.0412	0.0903	0.7216	0.075*
C3	0.1765 (4)	0.12135 (11)	0.7589 (4)	0.0499 (9)
H3	0.1875	0.1114	0.6591	0.060*
C4	0.2981 (4)	0.14907 (10)	0.8698 (4)	0.0355 (8)
C5	0.2811 (4)	0.16295 (11)	1.0175 (4)	0.0435 (8)
H5	0.3615	0.1813	1.0924	0.052*
C6	0.1457 (4)	0.14992 (11)	1.0563 (4)	0.0508 (9)
H6	0.1342	0.1590	1.1566	0.061*
C7	0.4382 (3)	0.16452 (11)	0.8228 (4)	0.0364 (8)
C8	0.4831 (4)	0.21105 (11)	0.8269 (4)	0.0393 (8)
C9	0.3873 (4)	0.24705 (13)	0.8674 (4)	0.0500 (9)
C10	0.6234 (4)	0.22698 (12)	0.7842 (4)	0.0496 (9)
C11	0.7833 (5)	0.29406 (14)	0.7680 (6)	0.0852 (14)
H11A	0.8090	0.2754	0.6845	0.102*
H11B	0.7593	0.3262	0.7265	0.102*

C12	0.9218 (6)	0.29404 (18)	0.9250 (7)	0.1152 (19)
H12A	0.8934	0.3111	1.0087	0.173*
H12B	1.0131	0.3091	0.9076	0.173*
H12C	0.9495	0.2620	0.9612	0.173*
C13	0.5356 (4)	0.08297 (11)	0.7983 (4)	0.0419 (8)
C14	0.6074 (3)	0.05767 (10)	0.6913 (4)	0.0368 (8)
C15	0.6086 (4)	0.06716 (10)	0.5305 (4)	0.0420 (8)
C16	0.6972 (4)	0.03064 (12)	0.4911 (4)	0.0474 (9)
C17	0.7410 (5)	0.02500 (13)	0.3371 (4)	0.0622 (11)
H17A	0.6468	0.0320	0.2399	0.075*
H17B	0.7720	−0.0077	0.3285	0.075*
C18	0.8792 (5)	0.05739 (14)	0.3384 (5)	0.0823 (13)
H18A	0.8501	0.0897	0.3500	0.123*
H18B	0.9005	0.0539	0.2356	0.123*
H18C	0.9747	0.0492	0.4304	0.123*
C19	0.7339 (4)	−0.00981 (12)	0.8945 (4)	0.0601 (10)
H19A	0.7329	−0.0433	0.8734	0.090*
H19B	0.6562	−0.0026	0.9480	0.090*
H19C	0.8402	−0.0005	0.9659	0.090*
Cl1	0.51799 (13)	0.11280 (3)	0.40193 (12)	0.0750 (4)
F1	−0.1038 (2)	0.11074 (8)	0.9808 (3)	0.0846 (7)
N1	0.3149 (4)	0.27709 (11)	0.8997 (4)	0.0712 (10)
N2	0.5170 (3)	0.13141 (9)	0.7615 (4)	0.0487 (8)
N3	0.6914 (3)	0.01611 (9)	0.7359 (3)	0.0437 (7)
N4	0.7463 (3)	0.00016 (9)	0.6167 (4)	0.0500 (7)
O1	0.7110 (3)	0.20129 (8)	0.7383 (3)	0.0681 (8)
O2	0.6422 (3)	0.27364 (8)	0.7995 (3)	0.0695 (8)
O3	0.4979 (3)	0.06497 (8)	0.9086 (3)	0.0570 (7)
H2A	0.584 (4)	0.1442 (11)	0.718 (4)	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.035 (2)	0.062 (2)	0.060 (3)	−0.0047 (18)	0.021 (2)	0.012 (2)
C2	0.043 (2)	0.082 (3)	0.056 (3)	−0.017 (2)	0.008 (2)	−0.006 (2)
C3	0.044 (2)	0.064 (2)	0.043 (2)	−0.0017 (18)	0.0162 (18)	−0.0029 (18)
C4	0.0298 (18)	0.0344 (17)	0.044 (2)	0.0045 (14)	0.0148 (16)	0.0057 (15)
C5	0.044 (2)	0.0418 (19)	0.048 (2)	−0.0061 (16)	0.0203 (17)	−0.0018 (16)
C6	0.048 (2)	0.057 (2)	0.053 (2)	−0.0006 (18)	0.025 (2)	0.0019 (19)
C7	0.0335 (18)	0.0372 (19)	0.039 (2)	0.0045 (15)	0.0138 (16)	0.0015 (15)
C8	0.0377 (19)	0.0390 (19)	0.044 (2)	−0.0014 (15)	0.0175 (16)	0.0023 (15)
C9	0.052 (2)	0.042 (2)	0.065 (3)	−0.0062 (18)	0.032 (2)	0.0070 (19)
C10	0.047 (2)	0.045 (2)	0.061 (3)	−0.0047 (18)	0.024 (2)	−0.0002 (18)
C11	0.083 (3)	0.071 (3)	0.125 (4)	−0.033 (2)	0.066 (3)	−0.018 (3)
C12	0.075 (4)	0.151 (5)	0.134 (5)	−0.038 (3)	0.055 (4)	−0.020 (4)
C13	0.0326 (19)	0.045 (2)	0.050 (2)	−0.0013 (15)	0.0154 (17)	−0.0003 (18)
C14	0.0333 (18)	0.0344 (18)	0.044 (2)	−0.0032 (15)	0.0141 (16)	−0.0027 (16)
C15	0.0384 (19)	0.0382 (19)	0.048 (2)	−0.0033 (15)	0.0123 (17)	0.0059 (17)

C16	0.049 (2)	0.045 (2)	0.049 (2)	−0.0045 (17)	0.0190 (18)	−0.0056 (18)
C17	0.077 (3)	0.063 (2)	0.057 (3)	−0.004 (2)	0.035 (2)	−0.011 (2)
C18	0.093 (3)	0.095 (3)	0.078 (3)	−0.007 (3)	0.053 (3)	−0.008 (3)
C19	0.073 (3)	0.053 (2)	0.059 (2)	0.0189 (19)	0.028 (2)	0.022 (2)
Cl1	0.0929 (8)	0.0713 (7)	0.0610 (7)	0.0272 (6)	0.0263 (6)	0.0243 (5)
F1	0.0501 (13)	0.125 (2)	0.0863 (17)	−0.0232 (13)	0.0327 (12)	0.0097 (14)
N1	0.080 (2)	0.051 (2)	0.101 (3)	0.0108 (18)	0.054 (2)	0.0082 (19)
N2	0.0528 (19)	0.0356 (17)	0.072 (2)	−0.0037 (14)	0.0398 (16)	0.0049 (15)
N3	0.0450 (17)	0.0389 (16)	0.0499 (18)	0.0085 (13)	0.0195 (14)	0.0048 (14)
N4	0.0513 (18)	0.0445 (17)	0.0588 (19)	0.0021 (14)	0.0246 (16)	−0.0079 (16)
O1	0.0695 (18)	0.0550 (16)	0.104 (2)	−0.0085 (14)	0.0615 (17)	−0.0030 (15)
O2	0.0747 (18)	0.0477 (15)	0.107 (2)	−0.0216 (13)	0.0577 (17)	−0.0145 (14)
O3	0.0658 (17)	0.0533 (15)	0.0635 (17)	0.0070 (12)	0.0370 (15)	0.0107 (13)

Geometric parameters (Å, °)

C1—C6	1.354 (4)	C12—H12B	0.9600
C1—C2	1.364 (5)	C12—H12C	0.9600
C1—F1	1.365 (3)	C13—O3	1.208 (4)
C2—C3	1.377 (4)	C13—N2	1.398 (4)
C2—H2	0.9300	C13—C14	1.458 (4)
C3—C4	1.398 (4)	C14—N3	1.367 (4)
C3—H3	0.9300	C14—C15	1.399 (4)
C4—C5	1.373 (4)	C15—C16	1.397 (4)
C4—C7	1.480 (4)	C15—Cl1	1.701 (3)
C5—C6	1.385 (4)	C16—N4	1.325 (4)
C5—H5	0.9300	C16—C17	1.495 (5)
C6—H6	0.9300	C17—C18	1.513 (5)
C7—N2	1.366 (4)	C17—H17A	0.9700
C7—C8	1.366 (4)	C17—H17B	0.9700
C8—C9	1.432 (5)	C18—H18A	0.9600
C8—C10	1.465 (4)	C18—H18B	0.9600
C9—N1	1.146 (4)	C18—H18C	0.9600
C10—O1	1.213 (4)	C19—N3	1.468 (4)
C10—O2	1.326 (4)	C19—H19A	0.9600
C11—C12	1.468 (6)	C19—H19B	0.9600
C11—O2	1.469 (4)	C19—H19C	0.9600
C11—H11A	0.9700	N2—H2A	0.87 (3)
C11—H11B	0.9700	N3—N4	1.340 (3)
C12—H12A	0.9600		
C6—C1—C2	123.9 (3)	H12B—C12—H12C	109.5
C6—C1—F1	118.4 (3)	O3—C13—N2	122.9 (3)
C2—C1—F1	117.7 (3)	O3—C13—C14	124.8 (3)
C1—C2—C3	117.5 (3)	N2—C13—C14	112.3 (3)
C1—C2—H2	121.2	N3—C14—C15	104.7 (3)
C3—C2—H2	121.2	N3—C14—C13	123.4 (3)
C2—C3—C4	120.9 (3)	C15—C14—C13	131.8 (3)
C2—C3—H3	119.6	C16—C15—C14	106.5 (3)
C4—C3—H3	119.6	C16—C15—Cl1	125.3 (3)

C5—C4—C3	118.9 (3)	C14—C15—Cl1	128.1 (3)
C5—C4—C7	121.5 (3)	N4—C16—C15	109.8 (3)
C3—C4—C7	119.6 (3)	N4—C16—C17	122.0 (3)
C4—C5—C6	120.8 (3)	C15—C16—C17	128.2 (3)
C4—C5—H5	119.6	C16—C17—C18	111.9 (3)
C6—C5—H5	119.6	C16—C17—H17A	109.2
C1—C6—C5	118.1 (3)	C18—C17—H17A	109.2
C1—C6—H6	121.0	C16—C17—H17B	109.2
C5—C6—H6	121.0	C18—C17—H17B	109.2
N2—C7—C8	119.2 (3)	H17A—C17—H17B	107.9
N2—C7—C4	118.4 (3)	C17—C18—H18A	109.5
C8—C7—C4	122.2 (3)	C17—C18—H18B	109.5
C7—C8—C9	120.0 (3)	H18A—C18—H18B	109.5
C7—C8—C10	123.1 (3)	C17—C18—H18C	109.5
C9—C8—C10	116.9 (3)	H18A—C18—H18C	109.5
N1—C9—C8	177.4 (4)	H18B—C18—H18C	109.5
O1—C10—O2	123.5 (3)	N3—C19—H19A	109.5
O1—C10—C8	125.0 (3)	N3—C19—H19B	109.5
O2—C10—C8	111.5 (3)	H19A—C19—H19B	109.5
C12—C11—O2	108.7 (4)	N3—C19—H19C	109.5
C12—C11—H11A	110.0	H19A—C19—H19C	109.5
O2—C11—H11A	110.0	H19B—C19—H19C	109.5
C12—C11—H11B	110.0	C7—N2—C13	128.1 (3)
O2—C11—H11B	110.0	C7—N2—H2A	112 (2)
H11A—C11—H11B	108.3	C13—N2—H2A	117 (2)
C11—C12—H12A	109.5	N4—N3—C14	112.0 (3)
C11—C12—H12B	109.5	N4—N3—C19	119.1 (3)
H12A—C12—H12B	109.5	C14—N3—C19	128.8 (3)
C11—C12—H12C	109.5	C16—N4—N3	107.0 (3)
H12A—C12—H12C	109.5	C10—O2—C11	117.1 (3)
C6—C1—C2—C3	−0.2 (6)	N3—C14—C15—C16	−1.2 (3)
F1—C1—C2—C3	−179.7 (3)	C13—C14—C15—C16	179.7 (3)
C1—C2—C3—C4	−0.6 (5)	N3—C14—C15—Cl1	177.4 (2)
C2—C3—C4—C5	0.8 (5)	C13—C14—C15—Cl1	−1.7 (5)
C2—C3—C4—C7	−176.6 (3)	C14—C15—C16—N4	0.7 (4)
C3—C4—C5—C6	−0.2 (5)	Cl1—C15—C16—N4	−177.9 (2)
C7—C4—C5—C6	177.1 (3)	C14—C15—C16—C17	−177.0 (3)
C2—C1—C6—C5	0.8 (5)	Cl1—C15—C16—C17	4.3 (5)
F1—C1—C6—C5	−179.7 (3)	N4—C16—C17—C18	−100.9 (4)
C4—C5—C6—C1	−0.6 (5)	C15—C16—C17—C18	76.6 (5)
C5—C4—C7—N2	134.2 (3)	C8—C7—N2—C13	154.6 (3)
C3—C4—C7—N2	−48.5 (4)	C4—C7—N2—C13	−30.3 (5)
C5—C4—C7—C8	−50.8 (4)	O3—C13—N2—C7	−9.2 (5)
C3—C4—C7—C8	126.5 (3)	C14—C13—N2—C7	171.9 (3)
N2—C7—C8—C9	170.9 (3)	C15—C14—N3—N4	1.3 (3)
C4—C7—C8—C9	−4.0 (5)	C13—C14—N3—N4	−179.5 (3)
N2—C7—C8—C10	−6.4 (5)	C15—C14—N3—C19	177.4 (3)
C4—C7—C8—C10	178.7 (3)	C13—C14—N3—C19	−3.4 (5)
C7—C8—C10—O1	1.6 (6)	C15—C16—N4—N3	0.1 (4)

C9—C8—C10—O1	−175.8 (3)	C17—C16—N4—N3	178.0 (3)
C7—C8—C10—O2	−179.4 (3)	C14—N3—N4—C16	−0.9 (3)
C9—C8—C10—O2	3.3 (4)	C19—N3—N4—C16	−177.4 (3)
O3—C13—C14—N3	−23.6 (5)	O1—C10—O2—C11	−3.8 (6)
N2—C13—C14—N3	155.2 (3)	C8—C10—O2—C11	177.2 (3)
O3—C13—C14—C15	155.3 (3)	C12—C11—O2—C10	−88.6 (4)
N2—C13—C14—C15	−25.8 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19B···O3	0.96	2.31	2.983 (4)	126
N2—H2A···O1	0.87 (3)	1.93 (3)	2.653 (3)	139 (3)
N2—H2A···Cl1	0.87 (3)	2.70 (3)	3.110 (3)	110 (3)

Fig. 1

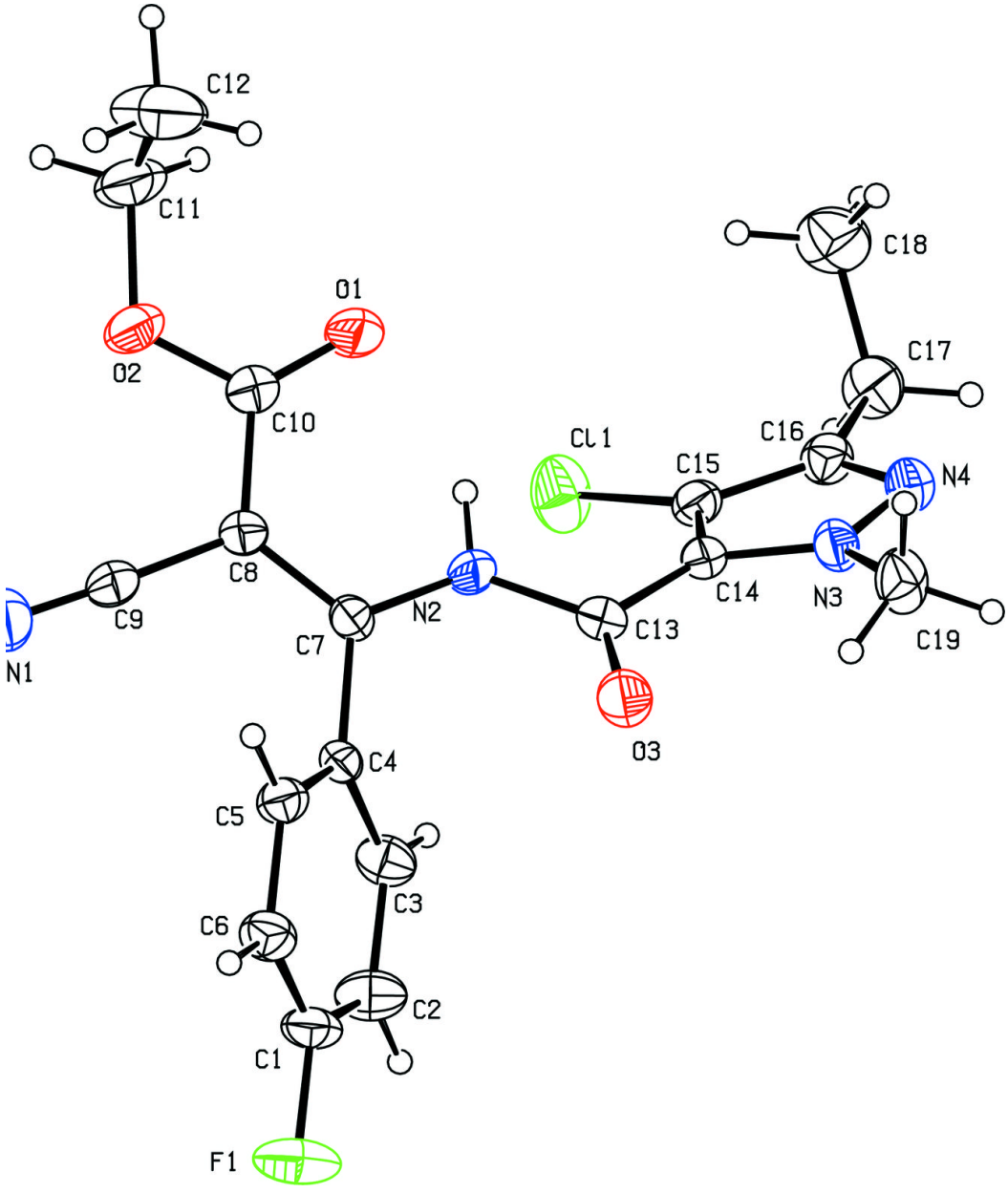
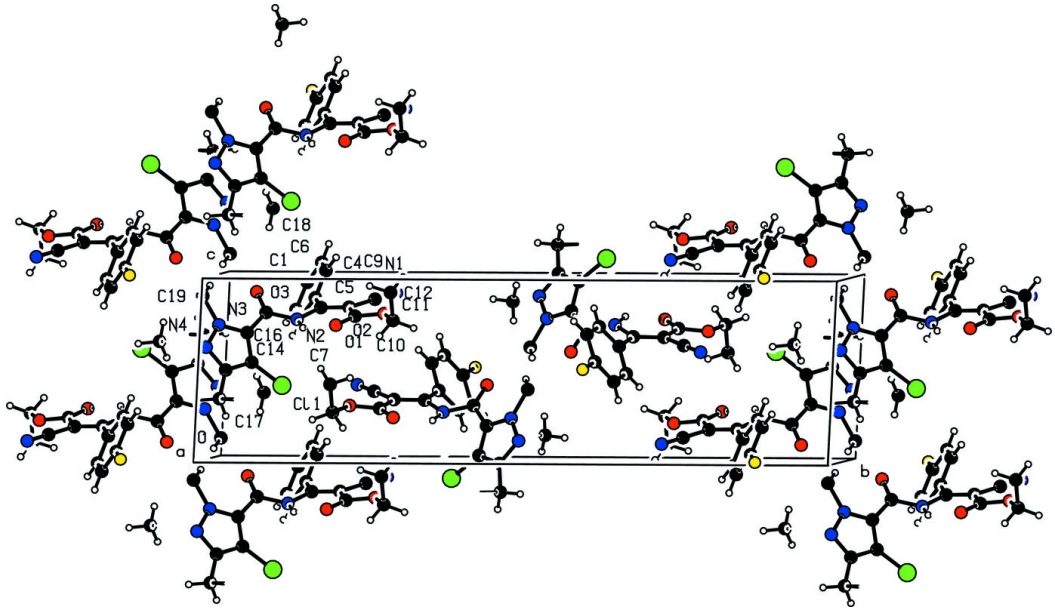

C12
C11
O1
O2
C10
C18
C17
C16
CL1
C15
N4
C8
C9
N1
N2
C7
C14
N3
C19
C13
O3
C4
C5
C3
C6
C2
C1
F1

Fig. 2


C18
C6
C1
C4
C9
N1
C19
O3
C5
C12
C11
N3
N4
C16
C14
N2
C7
O1
O2
C10
CL1
C17
O
c
a
b