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2-Ethoxy-3-(4-fluorophenyl)-4-oxo-5-phenyl-3,4-dihydro-5*H*-pyrrolo[3,2-*d*]-pyrimidine-7-carbonitrile

Ping He,[a] Xin-Min Peng[b] and Gui-Hua Li[a,c]*

[a]Key Laboratory of Pesticides and Chemical Biology, Ministry of Education, Central China Normal University, Wuhan 430079, People's Republic of China, [b]Taihe Hospital, Yunyang Medical College, Shiyan 442000, People's Republic of China, and [c]Department of Medicinal Chemistry, Yunyang Medical College, Shiyan 442000, People's Republic of China
Correspondence e-mail: ygh940802@yahoo.com.cn

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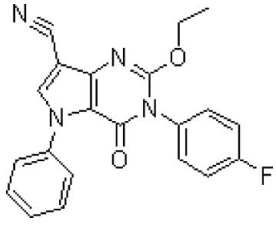
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.060; wR factor = 0.141; data-to-parameter ratio = 15.0.

In the crystal structure of the title compound, $C_{21}H_{15}FN_4O_2$, the two fused rings of pyrrolo[3,2-*d*]pyrimidine form a dihedral angle of 2.91 (12)°. The fluorophenyl and phenyl rings are twisted with respect to the heterocyclic pyrrolo[3,2-*d*]pyrimidine system, making dihedral angles of 75.23 (12) and 46.11 (14)°, respectively. The crystal packing is mainly stabilized by C—H···O and C—H···F hydrogen bonds, and π–π interactions with interplanar distances of 3.315 (1) Å between adjacent pyrrole ring centroids and 3.300 (1) Å between pyrrole and pyrimidinone rings. The ethyl group is disordered over two positions; the site occupancies are 0.65 and 0.35.

Related literature

Related preparation and biological activity are described by Shih *et al.* (2002) and Niwas *et al.* (1994). For related literature, see: Ding *et al.*, (2004); Hu *et al.* (2005, 2006); Janiak (2000).



Experimental

Crystal data

$C_{21}H_{15}FN_4O_2$
M_r = 374.37
Monoclinic, $P2_1/c$
a = 10.7513 (5) Å
b = 13.2684 (7) Å
c = 13.2210 (7) Å
β = 93.890 (1)°
V = 1881.66 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 273 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.981, T_{max} = 0.991
20895 measured reflections
4099 independent reflections
2039 reflections with $I > 2\sigma(I)$
R_{int} = 0.087

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.141
S = 0.90
4099 reflections
274 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 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
C6—H6···F1^{i}	0.93	2.49	3.306 (3)	146
C11—H11···O2^{i}	0.93	2.37	2.910 (3)	117

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2469).

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supplementary materials

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2-Ethoxy-3-(4-fluorophenyl)-4-oxo-5-phenyl-3,4-dihydro-5*H*-pyrrolo[3,2-*d*]pyrimidine-7-carbonitrile

P. He, X.-M. Peng and G.-H. Li

Comment

We have recently focused on the synthesis of fused heterocyclic systems containing a fused pyrimidinone unit using the aza-Wittig reaction (Ding *et al.*, 2004). Some X-ray crystal structures of fused pyrimidinone derivatives have been reported (Hu, Li *et al.*, 2005; Hu *et al.*, 2006). Pyrrolopyrimidine derivatives are of great importance because of their remarkable biological properties (Shih, *et al.*, 2002; Niwas, *et al.*, 1994). We present here the structure of one such pyrrolopyrimidine derivative, (I) (Fig. 1), which may be used as a new precursor for obtaining bioactive molecules.

The bond lengths and angles in (I) are unexceptional. The pyrrole (A), the pyrimidinone (B) and the C1—C6 benzene(C), the C14—C19 benzene(D) rings are, of course, planar and the dihedral angles between them are A/B = 2.91 (12)°, B/C = 75.23 (12)°, A/D = 46.11 (14)°. C20, C21 and attached hydrogen atoms are disordered over two sites, with refined occupancies of 0.65 (2) and 0.35 (2). Intermolecular C—H···O and C—H···F hydrogen bonds (Fig. 2 and Table 2) seem to be effective in stabilizing the crystal structure. Further stability is provided by offset π-π stacking interactions (Janiak, 2000) involving A and B rings. The A:A interplanar distance are 3.315 (1) Å with distances between adjacent ring centroids of 3.796 (1) Å. (symmetry code relating the adjacent rings: $1-x, -y, 1-z$). A further interaction occurs between two adjacent A and B rings (symmetry code: $1-x, -y, 1-z$), with an interplanar distance of 3.300 (1)Å and a centroid-to-centroid distance of 3.592 (1) (Fig. 2).

Experimental

To a solution of the ethyl 3-((4-fluorophenylimino)methyleneamino)- 4-cyano-1-phenyl-1*H*-pyrrole-2-carboxylate (II) (3 mmol) in dichloromethane (5 ml) was added sodium ethoxide(3 mmol)/ethanol (5 ml). After stirring the reaction mixture for 4 h, the solvent was removed under reduced pressure and the residue was recrystallized from ethanol to give the title compound, in a yield of 83%. Suitable crystals were obtained by vapour diffusion of ethanol into dichloromethane at room temperature.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å, U_{iso}=1.2U_{eq} (C) for C_{sp^2}, C—H = 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2, C—H = 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3. The relative occupancies for the disordered components were refined anisotropically to yield relative occupancies of 0.65 (2) and 0.35 (2), respectively, for C20, C21 and C20', C21'. The H atoms of these disorder atoms were located geometrically and refined using a riding model.

Figures

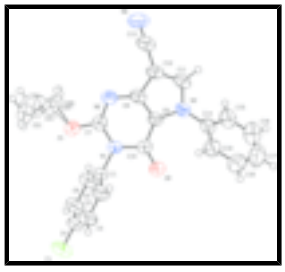


Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme. Only the major disorder component is shown.

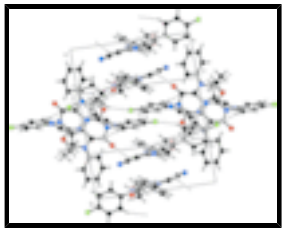


Fig. 2. The packing in the crystal structure, showing the C—H···O and C—H···F hydrogen bonds as dashed lines.

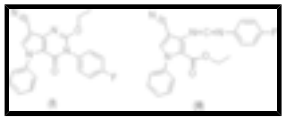


Fig. 3. The structures of (I) and (II).

2-Ethoxy-3-(4-fluorophenyl)-4-oxo-5-phenyl-3,4-dihydro-5*H*- pyrrolo[3,2-*d*]pyrimidine-7-carbonitrile

Crystal data

$C_{21}H_{15}FN_4O_2$	F_{000} = 776
M_r = 374.37	D_x = 1.322 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 543.0 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.7513 (5) Å	Cell parameters from 2131 reflections
b = 13.2684 (7) Å	θ = 2.2–21.9º
c = 13.2210 (7) Å	μ = 0.10 mm^{-1}
β = 93.890 (1)º	T = 273 (2) K
V = 1881.66 (17) Å^3	Block, colourless
Z = 4	0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer	4099 independent reflections
Radiation source: fine-focus sealed tube	2039 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.087
T = 298(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −13→13

T_{min} = 0.981, T_{max} = 0.991
20895 measured reflections
k = −16→16
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.141
S = 0.90
4099 reflections
274 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
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}	Occ. (<1)
C1	0.3122 (2)	0.13945 (18)	0.20338 (17)	0.0528 (6)	
C2	0.3710 (2)	0.0917 (2)	0.1285 (2)	0.0726 (8)	
H2	0.4348	0.0461	0.1451	0.087*	
C3	0.3351 (3)	0.1116 (2)	0.0277 (2)	0.0803 (8)	
H3	0.3756	0.0811	−0.0242	0.096*	
C4	0.2401 (3)	0.1761 (2)	0.00691 (19)	0.0698 (8)	
C5	0.1809 (3)	0.2252 (2)	0.0792 (2)	0.0756 (8)	
H5	0.1166	0.2702	0.0620	0.091*	
C6	0.2186 (2)	0.20656 (19)	0.17943 (18)	0.0673 (7)	
H6	0.1800	0.2398	0.2307	0.081*	
C7	0.2762 (2)	0.06506 (18)	0.3691 (2)	0.0572 (6)	
C8	0.3997 (2)	0.09608 (16)	0.50746 (16)	0.0481 (6)	
C9	0.4827 (2)	0.14991 (16)	0.45414 (16)	0.0464 (5)	
C10	0.4589 (2)	0.17129 (17)	0.34947 (17)	0.0519 (6)	
C11	0.5521 (2)	0.15273 (18)	0.61627 (18)	0.0561 (6)	

H11	0.6013	0.1657	0.6754	0.067*	
C12	0.4439 (2)	0.09814 (17)	0.61092 (16)	0.0516 (6)	
C13	0.3863 (2)	0.0526 (2)	0.6939 (2)	0.0617 (7)	
C14	0.6841 (2)	0.24385 (18)	0.50197 (17)	0.0549 (6)	
C15	0.7155 (2)	0.3248 (2)	0.5633 (2)	0.0727 (8)	
H15	0.6672	0.3410	0.6167	0.087*	
C16	0.8181 (3)	0.3818 (2)	0.5454 (3)	0.0946 (10)	
H16	0.8393	0.4367	0.5868	0.114*	
C17	0.8894 (3)	0.3581 (3)	0.4670 (3)	0.1001 (11)	
H17	0.9589	0.3970	0.4550	0.120*	
C18	0.8581 (3)	0.2764 (3)	0.4058 (2)	0.0899 (9)	
H18	0.9065	0.2605	0.3523	0.108*	
C19	0.7552 (2)	0.2182 (2)	0.4234 (2)	0.0697 (7)	
H19	0.7345	0.1626	0.3828	0.084*	
C20	0.0819 (10)	−0.0131 (13)	0.3779 (7)	0.083 (3)	0.65 (2)
H20A	0.0585	0.0380	0.4255	0.100*	0.65 (2)
H20B	0.1110	−0.0723	0.4155	0.100*	0.65 (2)
C21	−0.0264 (6)	−0.0390 (9)	0.3046 (6)	0.093 (3)	0.65 (2)
H21A	−0.0556	0.0210	0.2699	0.140*	0.65 (2)
H21B	−0.0924	−0.0672	0.3409	0.140*	0.65 (2)
H21C	−0.0003	−0.0871	0.2561	0.140*	0.65 (2)
C21'	−0.0320 (12)	0.0133 (19)	0.352 (2)	0.144 (8)	0.35 (2)
H21D	−0.0171	0.0747	0.3889	0.217*	0.35 (2)
H21E	−0.0945	−0.0255	0.3828	0.217*	0.35 (2)
H21F	−0.0603	0.0288	0.2831	0.217*	0.35 (2)
C20'	0.0904 (14)	−0.0484 (10)	0.3525 (19)	0.071 (5)	0.35 (2)
H20C	0.1168	−0.0708	0.4204	0.085*	0.35 (2)
H20D	0.0810	−0.1066	0.3082	0.085*	0.35 (2)
F1	0.20318 (17)	0.19477 (13)	−0.09212 (10)	0.1037 (6)	
N1	0.35061 (17)	0.12065 (14)	0.30899 (13)	0.0522 (5)	
N2	0.29355 (17)	0.05079 (14)	0.46511 (15)	0.0563 (5)	
N3	0.57688 (17)	0.18511 (14)	0.52239 (14)	0.0511 (5)	
N4	0.3401 (2)	0.01462 (19)	0.75895 (18)	0.0874 (8)	
O1	0.17933 (16)	0.02517 (14)	0.31431 (12)	0.0802 (6)	
O2	0.51702 (16)	0.22586 (14)	0.29545 (12)	0.0745 (5)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0566 (14)	0.0621 (15)	0.0395 (15)	−0.0110 (12)	0.0020 (12)	0.0040 (12)
C2	0.0683 (17)	0.099 (2)	0.0506 (18)	0.0091 (15)	0.0075 (14)	0.0043 (15)
C3	0.082 (2)	0.118 (2)	0.0420 (17)	−0.0072 (18)	0.0119 (15)	−0.0034 (16)
C4	0.081 (2)	0.090 (2)	0.0365 (16)	−0.0267 (17)	−0.0099 (14)	0.0092 (15)
C5	0.091 (2)	0.082 (2)	0.0516 (18)	0.0023 (16)	−0.0100 (15)	0.0057 (15)
C6	0.0823 (19)	0.0754 (18)	0.0436 (16)	0.0024 (15)	−0.0013 (14)	−0.0009 (13)
C7	0.0492 (14)	0.0687 (17)	0.0538 (17)	−0.0062 (12)	0.0028 (13)	0.0050 (13)
C8	0.0536 (14)	0.0525 (14)	0.0385 (14)	0.0102 (11)	0.0054 (11)	0.0006 (11)
C9	0.0500 (13)	0.0546 (14)	0.0352 (13)	0.0025 (11)	0.0061 (11)	0.0010 (11)

C10	0.0529 (14)	0.0586 (15)	0.0449 (15)	−0.0044 (12)	0.0070 (12)	0.0049 (12)
C11	0.0628 (16)	0.0669 (16)	0.0383 (15)	0.0127 (13)	0.0012 (12)	−0.0076 (12)
C12	0.0614 (15)	0.0572 (15)	0.0370 (15)	0.0143 (12)	0.0090 (12)	0.0021 (11)
C13	0.0693 (17)	0.0736 (18)	0.0426 (16)	0.0161 (14)	0.0059 (13)	0.0022 (14)
C14	0.0499 (14)	0.0617 (16)	0.0524 (16)	0.0040 (12)	−0.0020 (12)	−0.0027 (13)
C15	0.0681 (18)	0.0745 (19)	0.074 (2)	−0.0022 (15)	−0.0049 (15)	−0.0136 (15)
C16	0.081 (2)	0.090 (2)	0.110 (3)	−0.0136 (19)	−0.008 (2)	−0.016 (2)
C17	0.070 (2)	0.105 (3)	0.124 (3)	−0.0250 (19)	−0.002 (2)	0.001 (2)
C18	0.0674 (19)	0.118 (3)	0.086 (2)	−0.0061 (19)	0.0174 (16)	0.002 (2)
C19	0.0624 (17)	0.0803 (19)	0.0672 (19)	−0.0003 (15)	0.0091 (14)	−0.0061 (14)
C20	0.079 (5)	0.097 (7)	0.075 (6)	−0.040 (5)	0.008 (3)	0.015 (4)
C21	0.066 (4)	0.128 (7)	0.086 (5)	−0.029 (4)	0.003 (3)	0.002 (4)
C21'	0.128 (12)	0.163 (17)	0.14 (2)	0.022 (11)	0.029 (13)	0.018 (12)
C20'	0.073 (8)	0.087 (10)	0.053 (9)	−0.025 (6)	0.003 (6)	0.004 (7)
F1	0.1247 (14)	0.1418 (15)	0.0421 (10)	−0.0247 (12)	−0.0131 (9)	0.0147 (9)
N1	0.0524 (11)	0.0683 (13)	0.0360 (11)	−0.0075 (10)	0.0041 (9)	0.0083 (9)
N2	0.0607 (13)	0.0673 (13)	0.0412 (13)	0.0002 (10)	0.0060 (10)	0.0094 (10)
N3	0.0542 (12)	0.0605 (12)	0.0385 (12)	0.0025 (10)	0.0020 (9)	−0.0033 (9)
N4	0.0942 (18)	0.112 (2)	0.0575 (16)	0.0063 (14)	0.0210 (14)	0.0230 (14)
O1	0.0692 (12)	0.1153 (15)	0.0552 (12)	−0.0358 (11)	−0.0027 (10)	0.0205 (10)
O2	0.0754 (12)	0.0968 (13)	0.0505 (11)	−0.0280 (10)	−0.0012 (9)	0.0203 (10)

Geometric parameters (Å, °)

C1—C6	1.365 (3)	C14—C15	1.374 (3)
C1—C2	1.366 (3)	C14—C19	1.374 (3)
C1—N1	1.451 (3)	C14—N3	1.432 (3)
C2—C3	1.388 (3)	C15—C16	1.371 (4)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.346 (4)	C16—C17	1.367 (4)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.352 (4)	C17—C18	1.381 (4)
C4—F1	1.365 (3)	C17—H17	0.9300
C5—C6	1.381 (3)	C18—C19	1.382 (4)
C5—H5	0.9300	C18—H18	0.9300
C6—H6	0.9300	C19—H19	0.9300
C7—N2	1.284 (3)	C20—O1	1.477 (6)
C7—O1	1.337 (3)	C20—C21	1.504 (8)
C7—N1	1.379 (3)	C20—H20A	0.9700
C8—N2	1.374 (3)	C20—H20B	0.9700
C8—C9	1.375 (3)	C21—H21A	0.9600
C8—C12	1.418 (3)	C21—H21B	0.9600
C9—N3	1.390 (3)	C21—H21C	0.9600
C9—C10	1.419 (3)	C21'—C20'	1.549 (10)
C10—O2	1.219 (2)	C21'—H21D	0.9600
C10—N1	1.417 (3)	C21'—H21E	0.9600
C11—N3	1.357 (3)	C21'—H21F	0.9600
C11—C12	1.368 (3)	C20'—O1	1.480 (9)
C11—H11	0.9300	C20'—H20C	0.9700

C12—C13	1.429 (3)	C20'—H20D	0.9700
C13—N4	1.140 (3)		
C6—C1—C2	120.3 (2)	C14—C15—H15	120.1
C6—C1—N1	119.5 (2)	C17—C16—C15	120.2 (3)
C2—C1—N1	120.1 (2)	C17—C16—H16	119.9
C1—C2—C3	119.7 (3)	C15—C16—H16	119.9
C1—C2—H2	120.1	C16—C17—C18	119.9 (3)
C3—C2—H2	120.1	C16—C17—H17	120.1
C4—C3—C2	118.3 (3)	C18—C17—H17	120.1
C4—C3—H3	120.8	C17—C18—C19	120.4 (3)
C2—C3—H3	120.8	C17—C18—H18	119.8
C3—C4—C5	123.3 (2)	C19—C18—H18	119.8
C3—C4—F1	118.6 (3)	C14—C19—C18	118.8 (3)
C5—C4—F1	118.1 (3)	C14—C19—H19	120.6
C4—C5—C6	118.1 (3)	C18—C19—H19	120.6
C4—C5—H5	121.0	O1—C20—C21	105.0 (6)
C6—C5—H5	121.0	O1—C20—H20A	110.7
C1—C6—C5	120.2 (2)	C21—C20—H20A	110.7
C1—C6—H6	119.9	O1—C20—H20B	110.7
C5—C6—H6	119.9	C21—C20—H20B	110.7
N2—C7—O1	122.2 (2)	H20A—C20—H20B	108.8
N2—C7—N1	126.7 (2)	C20'—C21'—H21D	109.5
O1—C7—N1	111.1 (2)	C20'—C21'—H21E	109.5
N2—C8—C9	124.6 (2)	H21D—C21'—H21E	109.5
N2—C8—C12	128.0 (2)	C20'—C21'—H21F	109.5
C9—C8—C12	107.3 (2)	H21D—C21'—H21F	109.5
C8—C9—N3	108.15 (19)	H21E—C21'—H21F	109.5
C8—C9—C10	121.6 (2)	O1—C20'—C21'	102.6 (8)
N3—C9—C10	129.9 (2)	O1—C20'—H20C	111.3
O2—C10—N1	120.1 (2)	C21'—C20'—H20C	111.3
O2—C10—C9	128.6 (2)	O1—C20'—H20D	111.3
N1—C10—C9	111.3 (2)	C21'—C20'—H20D	111.3
N3—C11—C12	109.8 (2)	H20C—C20'—H20D	109.2
N3—C11—H11	125.1	C7—N1—C10	121.96 (19)
C12—C11—H11	125.1	C7—N1—C1	120.56 (18)
C11—C12—C8	106.8 (2)	C10—N1—C1	117.07 (17)
C11—C12—C13	126.5 (2)	C7—N2—C8	113.5 (2)
C8—C12—C13	126.7 (2)	C11—N3—C9	107.92 (19)
N4—C13—C12	178.7 (3)	C11—N3—C14	123.73 (19)
C15—C14—C19	120.8 (2)	C9—N3—C14	128.34 (19)
C15—C14—N3	118.9 (2)	C7—O1—C20	112.6 (4)
C19—C14—N3	120.3 (2)	C7—O1—C20'	125.0 (10)
C16—C15—C14	119.9 (3)	C20—O1—C20'	22.9 (7)
C16—C15—H15	120.1		
C6—C1—C2—C3	−0.1 (4)	N2—C7—N1—C10	−0.7 (4)
N1—C1—C2—C3	−178.8 (2)	O1—C7—N1—C10	179.49 (19)
C1—C2—C3—C4	−1.7 (4)	N2—C7—N1—C1	−173.2 (2)
C2—C3—C4—C5	2.4 (4)	O1—C7—N1—C1	7.0 (3)

C2—C3—C4—F1	−179.1 (2)	O2—C10—N1—C7	−174.4 (2)
C3—C4—C5—C6	−1.2 (4)	C9—C10—N1—C7	4.6 (3)
F1—C4—C5—C6	−179.8 (2)	O2—C10—N1—C1	−1.7 (3)
C2—C1—C6—C5	1.3 (4)	C9—C10—N1—C1	177.32 (19)
N1—C1—C6—C5	−180.0 (2)	C6—C1—N1—C7	73.3 (3)
C4—C5—C6—C1	−0.7 (4)	C2—C1—N1—C7	−108.0 (3)
N2—C8—C9—N3	179.27 (19)	C6—C1—N1—C10	−99.5 (3)
C12—C8—C9—N3	−0.1 (2)	C2—C1—N1—C10	79.2 (3)
N2—C8—C9—C10	6.0 (3)	O1—C7—N2—C8	178.6 (2)
C12—C8—C9—C10	−173.36 (19)	N1—C7—N2—C8	−1.1 (3)
C8—C9—C10—O2	172.0 (2)	C9—C8—N2—C7	−1.5 (3)
N3—C9—C10—O2	0.3 (4)	C12—C8—N2—C7	177.7 (2)
C8—C9—C10—N1	−7.0 (3)	C12—C11—N3—C9	−0.5 (2)
N3—C9—C10—N1	−178.7 (2)	C12—C11—N3—C14	−179.63 (19)
N3—C11—C12—C8	0.4 (2)	C8—C9—N3—C11	0.3 (2)
N3—C11—C12—C13	−179.2 (2)	C10—C9—N3—C11	172.9 (2)
N2—C8—C12—C11	−179.5 (2)	C8—C9—N3—C14	179.4 (2)
C9—C8—C12—C11	−0.2 (2)	C10—C9—N3—C14	−8.0 (4)
N2—C8—C12—C13	0.1 (4)	C15—C14—N3—C11	−46.1 (3)
C9—C8—C12—C13	179.4 (2)	C19—C14—N3—C11	132.7 (2)
C11—C12—C13—N4	−135 (12)	C15—C14—N3—C9	134.9 (2)
C8—C12—C13—N4	46 (12)	C19—C14—N3—C9	−46.3 (3)
C19—C14—C15—C16	0.8 (4)	N2—C7—O1—C20	14.4 (9)
N3—C14—C15—C16	179.6 (2)	N1—C7—O1—C20	−165.8 (8)
C14—C15—C16—C17	−0.1 (4)	N2—C7—O1—C20'	−7.7 (8)
C15—C16—C17—C18	−0.2 (5)	N1—C7—O1—C20'	172.1 (7)
C16—C17—C18—C19	−0.2 (5)	C21—C20—O1—C7	171.1 (11)
C15—C14—C19—C18	−1.2 (4)	C21—C20—O1—C20'	−61 (3)
N3—C14—C19—C18	−180.0 (2)	C21'—C20'—O1—C7	112 (2)
C17—C18—C19—C14	0.8 (4)	C21'—C20'—O1—C20	49 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···F1^{i}	0.93	2.49	3.306 (3)	146
C11—H11···O2^{i}	0.93	2.37	2.910 (3)	117

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

Fig. 1

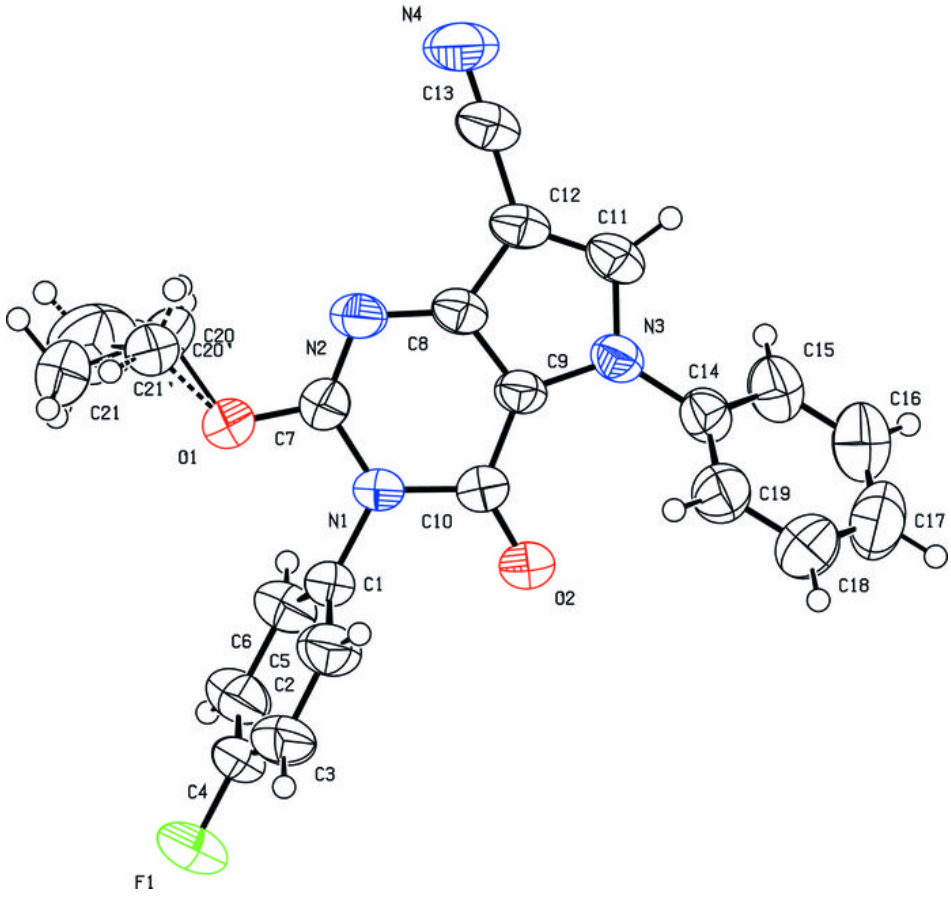

N4
C13
C12
C11
N3
C15
C16
C14
C9
C8
N2
C20
C20'
C21'
C21
O1
C7
N1
C10
O2
C19
C17
C18
C1
C6
C5
C2
C3
C4
F1

Fig. 2

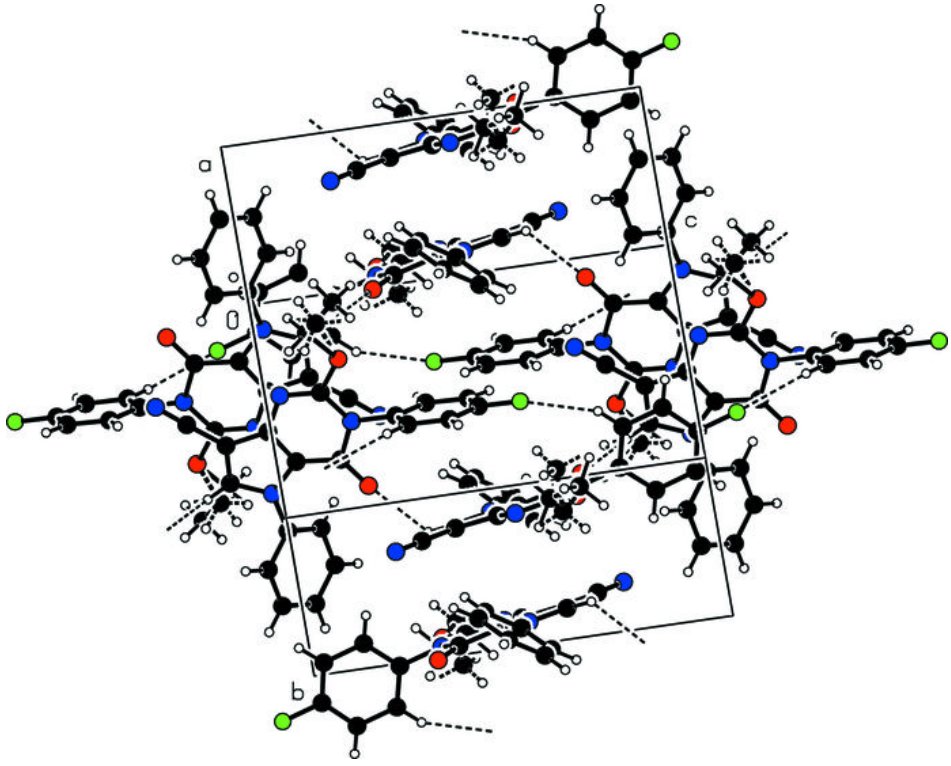
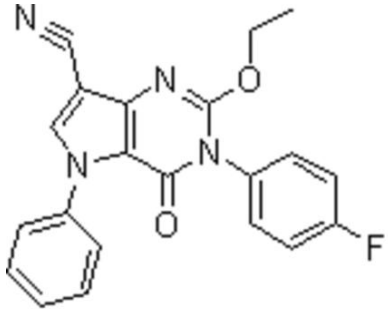
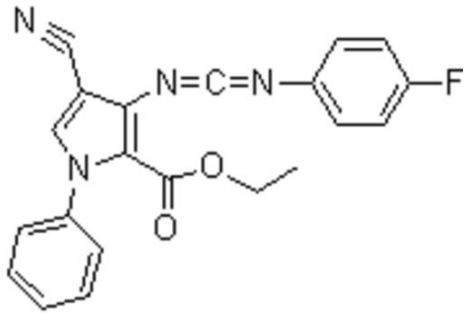


Fig. 3



(I)



(II)