Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 1-(2,6-difluorobenzyl)-4-(4,6-dimethoxypyrimidin-2-yl)-2-oxo-1,2-dihydroquinoline-3-carboxylate

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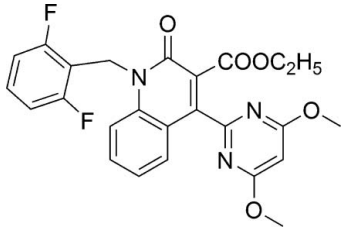
Received 12 November 2007; accepted 18 November 2007

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.053; wR factor = 0.140; data-to-parameter ratio = 16.2.

In the title compound, $C_{25}H_{21}F_2N_3O_5$, the quinoline unit is almost planar, with a maximum deviation of 0.076 (2) Å. The quinoline plane makes dihedral angles of 53.94 (5) and 85.79 (5)° with the pyrimidine and benzene rings, respectively. In the crystal structure, intermolecular C—H···O hydrogen bonds form a centrosymmetric dimer. The ethyl group is disordered over two positions, with occupancy factors of 0.778 (16) and 0.222 (16).

Related literature

For related literature, see: Duggleby & Pang (2000); Li & Luo (2006); Li & Wang (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{25}H_{21}F_2N_3O_5$
M_r = 481.45
Orthorhombic, *Pbca*
a = 11.667 (2) Å
b = 15.686 (3) Å
c = 24.594 (5) Å
V = 4500.9 (15) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 299 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
41620 measured reflections
5503 independent reflections
4211 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.140
S = 1.04
5503 reflections
339 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 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
C19—H19A···O5	0.97	2.25	2.665 (2)	105
C14—H14···N1	0.93	2.51	3.064 (2)	119
C23—H23···O4^{i}	0.93	2.52	3.288 (3)	140

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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* (Bruker, 2001).

The authors are indebted to Professor Guang-Fu Yang. This work was supported by the National 973 Project (2003CB114400), the National Natural Science Foundation of China (Nos. 20572030, 20528201 and 20432010), the Key Project of the Ministry of Education (Nos. 103116 and 104205), and the Program for Excellent Research Groups of Hubei Province (No. 2004ABC002).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2246).

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supplementary materials

Acta Cryst. (2007). E**63**, o4855 [**doi:10.1107/S1600536807060345**]

Ethyl 1-(2,6-difluorobenzyl)-4-(4,6-dimethoxypyrimidin-2-yl)-2-oxo-1,2-dihydroquinoline-3-carboxylate

Y.-X. Li, D.-Z. Chen and X.-J. Gong

Comment

Pyrimidine derivatives have broad biological properties; in particular pyrimidinylbenzoates are highly effective herbicides with acetohydroxyacid synthase (AHAS) as target (Duggleby & Pang, 2000). We herein report the crystal structure of one such pyrimidine derivative, the title compound, (I). In the molecule of (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). The quinoline fused rings (N3/C7—C15) are almost planar with a maximum deviation of 0.076 (2) Å for C9. Pyrimidine ring A (N1—N2/C3—C6) and quinoline ring B (N3/C7—C15) are nearly vertical with the dihedral angle [53.94 (5)°]. Similarly, quinoline ring B (N3/C7—C15) and the benzene ring C (C20—C25) are nearly vertical with the dihedral angle [85.79 (5)°]. In the crystal of (I), intermolecular C—H···O hydrogen bonds (Table 1) form a centrosymmetric dimer (Fig. 2).

Experimental

The title compound was synthesized according to the literature method (Li & Wang, 2007). Crystals appropriate for X-ray data collection were obtained by slow evaporation of the dichloromethane solution at 283 K.

Refinement

The ethyl group was disordered over two positions and the final occupancies for the major and minor disorder components refined to 0.778 (16) and 0.222 (16), respectively. All H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

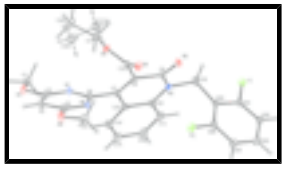

Fig. 1. The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

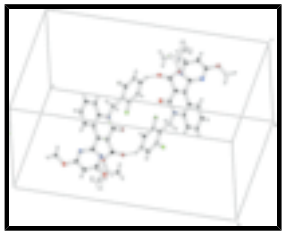

Fig. 2. A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

Ethyl 1-(2,6-difluorobenzyl)-4-(4,6-dimethoxypyrimidin-2-yl)-2-oxo- 1,2-dihydroquinoline-3-carboxylate

Crystal data

$C_{25}H_{21}F_2N_3O_5$	F_{000} = 2000
M_r = 481.45	D_x = 1.421 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 9565 reflections
a = 11.667 (2) Å	θ = 2.3–26.6º
b = 15.686 (3) Å	μ = 0.11 mm^{-1}
c = 24.594 (5) Å	*T* = 299 (2) K
V = 4500.9 (15) Å^3	Block, colorless
Z = 8	0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer	4211 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.032
Monochromator: graphite	θ_{max} = 28.3º
T = 299(2) K	θ_{min} = 1.7º
φ and ω scans	*h* = −15→15
Absorption correction: none	*k* = −20→20
41620 measured reflections	*l* = −32→32
5503 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
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.140	$w = 1/[\sigma^2(F_o^2) + (0.0676P)^2 + 1.2956P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
5503 reflections	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
339 parameters	$\Delta\rho_{min}$ = −0.21 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}	Occ. (<1)
C1	0.73891 (17)	0.17372 (13)	0.16587 (7)	0.0539 (4)	
H1A	0.6826	0.1346	0.1796	0.081*	
H1B	0.7616	0.1566	0.1300	0.081*	
H1C	0.7069	0.2301	0.1645	0.081*	
C2	0.96976 (18)	0.27238 (15)	0.42359 (8)	0.0632 (5)	
H2A	0.9374	0.3286	0.4237	0.095*	
H2B	1.0404	0.2726	0.4436	0.095*	
H2C	0.9170	0.2333	0.4403	0.095*	
C3	0.82340 (14)	0.20613 (11)	0.25095 (7)	0.0444 (4)	
C4	0.91887 (15)	0.21000 (13)	0.28369 (7)	0.0525 (5)	
H4	0.9905	0.1916	0.2719	0.063*	
C5	0.90176 (14)	0.24282 (12)	0.33494 (7)	0.0456 (4)	
C6	0.71497 (13)	0.26394 (10)	0.31678 (6)	0.0355 (3)	
C7	0.60120 (12)	0.29476 (10)	0.33717 (6)	0.0345 (3)	
C8	0.56031 (13)	0.26459 (9)	0.38473 (6)	0.0357 (3)	
C9	0.45379 (13)	0.29613 (10)	0.40849 (7)	0.0399 (4)	
C10	0.43375 (13)	0.38819 (10)	0.32902 (6)	0.0403 (4)	
C11	0.37353 (17)	0.45238 (12)	0.30178 (8)	0.0548 (5)	
H11	0.3036	0.4711	0.3154	0.066*	
C12	0.4169 (2)	0.48787 (14)	0.25515 (8)	0.0680 (6)	
H12	0.3759	0.5304	0.2374	0.082*	
C13	0.5208 (2)	0.46126 (14)	0.23429 (8)	0.0683 (6)	
H13	0.5498	0.4859	0.2028	0.082*	
C14	0.58106 (17)	0.39824 (12)	0.26040 (7)	0.0527 (4)	
H14	0.6510	0.3805	0.2462	0.063*	
C15	0.53945 (13)	0.36009 (10)	0.30785 (6)	0.0381 (3)	
C16	0.62206 (14)	0.19825 (11)	0.41763 (7)	0.0416 (4)	
C17	0.7161 (6)	0.0662 (3)	0.41641 (15)	0.0577 (13)	0.778 (16)
H17A	0.7833	0.0943	0.4311	0.069*	0.778 (16)
H17B	0.6744	0.0400	0.4462	0.069*	0.778 (16)
C18	0.7505 (7)	0.0008 (4)	0.37631 (18)	0.091 (2)	0.778 (16)
H18A	0.6833	−0.0250	0.3609	0.137*	0.778 (16)
H18B	0.7957	−0.0422	0.3940	0.137*	0.778 (16)
H18C	0.7948	0.0270	0.3480	0.137*	0.778 (16)
C19	0.28061 (13)	0.37913 (11)	0.39887 (8)	0.0489 (4)	
H19A	0.2558	0.3362	0.4247	0.059*	
H19B	0.2259	0.3793	0.3692	0.059*	
C20	0.27564 (14)	0.46494 (10)	0.42655 (6)	0.0411 (4)	

C21	0.16912 (15)	0.50102 (11)	0.43621 (7)	0.0477 (4)	
C22	0.15155 (17)	0.57584 (12)	0.46330 (8)	0.0554 (5)	
H22	0.0779	0.5968	0.4687	0.066*	
C23	0.24528 (19)	0.61930 (12)	0.48243 (7)	0.0567 (5)	
H23	0.2354	0.6702	0.5013	0.068*	
C24	0.35306 (18)	0.58806 (12)	0.47389 (8)	0.0553 (5)	
H24	0.4169	0.6176	0.4865	0.066*	
C25	0.36606 (15)	0.51210 (12)	0.44638 (7)	0.0485 (4)	
C17'	0.6721 (18)	0.0438 (12)	0.4027 (10)	0.072 (5)	0.222 (16)
H17C	0.6256	0.0023	0.3835	0.086*	0.222 (16)
H17D	0.6648	0.0348	0.4416	0.086*	0.222 (16)
C18'	0.7912 (17)	0.0403 (15)	0.3854 (11)	0.098 (7)	0.222 (16)
H18D	0.7949	0.0432	0.3465	0.146*	0.222 (16)
H18E	0.8249	−0.0121	0.3976	0.146*	0.222 (16)
H18F	0.8323	0.0875	0.4008	0.146*	0.222 (16)
F1	0.07698 (9)	0.45818 (8)	0.41673 (6)	0.0764 (4)	
F2	0.47380 (9)	0.48299 (8)	0.43831 (6)	0.0781 (4)	
N1	0.71969 (11)	0.23260 (9)	0.26652 (5)	0.0398 (3)	
N2	0.80033 (11)	0.27073 (9)	0.35220 (5)	0.0404 (3)	
N3	0.39250 (11)	0.35336 (8)	0.37715 (6)	0.0411 (3)	
O1	0.83663 (11)	0.17355 (10)	0.20088 (5)	0.0589 (4)	
O2	0.99134 (10)	0.24637 (11)	0.36873 (5)	0.0644 (4)	
O3	0.64202 (11)	0.12895 (7)	0.38783 (5)	0.0528 (3)	
O4	0.64791 (13)	0.20567 (9)	0.46424 (5)	0.0620 (4)	
O5	0.41807 (11)	0.27281 (9)	0.45267 (5)	0.0591 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0625 (11)	0.0618 (11)	0.0375 (8)	−0.0010 (9)	0.0005 (8)	−0.0063 (8)
C2	0.0535 (11)	0.0886 (16)	0.0475 (10)	−0.0034 (11)	−0.0107 (9)	−0.0078 (10)
C3	0.0446 (9)	0.0534 (10)	0.0352 (8)	0.0105 (7)	0.0062 (7)	0.0002 (7)
C4	0.0369 (9)	0.0769 (13)	0.0436 (9)	0.0160 (8)	0.0074 (7)	0.0013 (9)
C5	0.0341 (8)	0.0624 (11)	0.0402 (8)	0.0039 (7)	0.0010 (6)	0.0029 (7)
C6	0.0333 (7)	0.0383 (8)	0.0349 (7)	0.0014 (6)	0.0046 (6)	0.0003 (6)
C7	0.0316 (7)	0.0365 (8)	0.0355 (7)	0.0002 (6)	0.0008 (6)	−0.0059 (6)
C8	0.0345 (7)	0.0345 (8)	0.0382 (7)	−0.0006 (6)	0.0035 (6)	−0.0057 (6)
C9	0.0381 (8)	0.0352 (8)	0.0465 (8)	−0.0028 (6)	0.0084 (7)	−0.0069 (7)
C10	0.0407 (8)	0.0384 (8)	0.0418 (8)	0.0030 (7)	−0.0051 (7)	−0.0110 (6)
C11	0.0540 (10)	0.0578 (11)	0.0527 (10)	0.0195 (9)	−0.0095 (8)	−0.0114 (9)
C12	0.0888 (16)	0.0636 (12)	0.0516 (11)	0.0312 (12)	−0.0163 (11)	0.0006 (9)
C13	0.0909 (16)	0.0662 (13)	0.0478 (10)	0.0181 (12)	0.0046 (10)	0.0130 (9)
C14	0.0602 (11)	0.0539 (10)	0.0438 (9)	0.0093 (9)	0.0055 (8)	0.0037 (8)
C15	0.0382 (8)	0.0388 (8)	0.0372 (7)	0.0017 (6)	−0.0019 (6)	−0.0052 (6)
C16	0.0405 (8)	0.0428 (9)	0.0416 (9)	0.0033 (7)	0.0095 (7)	0.0020 (7)
C17	0.080 (3)	0.043 (2)	0.0501 (17)	0.0207 (18)	−0.0069 (17)	0.0038 (13)
C18	0.134 (5)	0.062 (3)	0.078 (2)	0.054 (3)	−0.016 (3)	−0.014 (2)
C19	0.0325 (8)	0.0458 (9)	0.0683 (11)	0.0029 (7)	0.0065 (8)	−0.0154 (8)

C20	0.0416 (9)	0.0386 (8)	0.0432 (8)	0.0062 (7)	0.0061 (7)	−0.0025 (7)
C21	0.0444 (9)	0.0444 (9)	0.0544 (10)	0.0056 (7)	0.0104 (8)	0.0009 (8)
C22	0.0597 (11)	0.0488 (10)	0.0576 (11)	0.0190 (9)	0.0147 (9)	0.0008 (8)
C23	0.0831 (14)	0.0424 (9)	0.0445 (9)	0.0154 (10)	0.0040 (9)	−0.0048 (7)
C24	0.0676 (12)	0.0485 (10)	0.0497 (10)	0.0000 (9)	−0.0101 (9)	−0.0066 (8)
C25	0.0443 (9)	0.0505 (10)	0.0508 (9)	0.0072 (8)	−0.0035 (7)	−0.0068 (8)
C17'	0.074 (10)	0.060 (8)	0.082 (11)	0.000 (7)	−0.006 (7)	0.013 (7)
C18'	0.089 (11)	0.053 (10)	0.150 (17)	0.027 (8)	−0.007 (10)	0.012 (10)
F1	0.0377 (6)	0.0686 (8)	0.1229 (11)	0.0027 (5)	0.0088 (6)	−0.0205 (7)
F2	0.0420 (6)	0.0805 (9)	0.1117 (10)	0.0073 (6)	−0.0124 (6)	−0.0393 (8)
N1	0.0365 (7)	0.0483 (8)	0.0347 (6)	0.0055 (6)	0.0031 (5)	−0.0023 (5)
N2	0.0349 (7)	0.0502 (8)	0.0359 (7)	0.0013 (6)	0.0021 (5)	−0.0017 (6)
N3	0.0336 (7)	0.0388 (7)	0.0509 (8)	0.0039 (5)	0.0057 (6)	−0.0100 (6)
O1	0.0547 (7)	0.0840 (10)	0.0380 (6)	0.0219 (7)	0.0051 (5)	−0.0110 (6)
O2	0.0359 (6)	0.1100 (12)	0.0473 (7)	0.0091 (7)	−0.0039 (5)	−0.0059 (7)
O3	0.0692 (8)	0.0393 (6)	0.0500 (7)	0.0133 (6)	0.0068 (6)	0.0023 (5)
O4	0.0743 (9)	0.0713 (9)	0.0404 (7)	0.0147 (7)	−0.0015 (6)	0.0008 (6)
O5	0.0556 (8)	0.0628 (8)	0.0589 (8)	0.0052 (6)	0.0257 (6)	0.0083 (6)

Geometric parameters (Å, °)

C1—O1	1.429 (2)	C14—C15	1.398 (2)
C1—H1A	0.9600	C14—H14	0.9300
C1—H1B	0.9600	C16—O4	1.191 (2)
C1—H1C	0.9600	C16—O3	1.332 (2)
C2—O2	1.432 (2)	C17—C18	1.479 (6)
C2—H2A	0.9600	C17—O3	1.487 (4)
C2—H2B	0.9600	C17—H17A	0.9700
C2—H2C	0.9600	C17—H17B	0.9700
C3—N1	1.335 (2)	C18—H18A	0.9600
C3—O1	1.342 (2)	C18—H18B	0.9600
C3—C4	1.376 (2)	C18—H18C	0.9600
C4—C5	1.376 (2)	C19—N3	1.467 (2)
C4—H4	0.9300	C19—C20	1.509 (2)
C5—N2	1.331 (2)	C19—H19A	0.9700
C5—O2	1.336 (2)	C19—H19B	0.9700
C6—N2	1.327 (2)	C20—C25	1.378 (2)
C6—N1	1.3314 (19)	C20—C21	1.386 (2)
C6—C7	1.499 (2)	C21—F1	1.355 (2)
C7—C8	1.349 (2)	C21—C22	1.365 (3)
C7—C15	1.445 (2)	C22—C23	1.372 (3)
C8—C9	1.460 (2)	C22—H22	0.9300
C8—C16	1.502 (2)	C23—C24	1.366 (3)
C9—O5	1.220 (2)	C23—H23	0.9300
C9—N3	1.382 (2)	C24—C25	1.379 (3)
C10—N3	1.390 (2)	C24—H24	0.9300
C10—C11	1.399 (2)	C25—F2	1.352 (2)
C10—C15	1.409 (2)	C17'—O3	1.428 (15)
C11—C12	1.372 (3)	C17'—C18'	1.45 (3)

C11—H11	0.9300	C17'—H17C	0.9700
C12—C13	1.381 (3)	C17'—H17D	0.9700
C12—H12	0.9300	C18'—H18D	0.9600
C13—C14	1.372 (3)	C18'—H18E	0.9600
C13—H13	0.9300	C18'—H18F	0.9600
O1—C1—H1A	109.5	O3—C16—C8	110.66 (14)
O1—C1—H1B	109.5	C18—C17—O3	107.6 (3)
H1A—C1—H1B	109.5	C18—C17—H17A	110.2
O1—C1—H1C	109.5	O3—C17—H17A	110.2
H1A—C1—H1C	109.5	C18—C17—H17B	110.2
H1B—C1—H1C	109.5	O3—C17—H17B	110.2
O2—C2—H2A	109.5	H17A—C17—H17B	108.5
O2—C2—H2B	109.5	N3—C19—C20	116.36 (14)
H2A—C2—H2B	109.5	N3—C19—H19A	108.2
O2—C2—H2C	109.5	C20—C19—H19A	108.2
H2A—C2—H2C	109.5	N3—C19—H19B	108.2
H2B—C2—H2C	109.5	C20—C19—H19B	108.2
N1—C3—O1	119.06 (15)	H19A—C19—H19B	107.4
N1—C3—C4	123.51 (15)	C25—C20—C21	113.99 (15)
O1—C3—C4	117.42 (15)	C25—C20—C19	127.53 (15)
C3—C4—C5	115.79 (15)	C21—C20—C19	118.41 (15)
C3—C4—H4	122.1	F1—C21—C22	118.67 (16)
C5—C4—H4	122.1	F1—C21—C20	116.62 (15)
N2—C5—O2	118.89 (15)	C22—C21—C20	124.71 (18)
N2—C5—C4	122.96 (15)	C21—C22—C23	118.35 (17)
O2—C5—C4	118.15 (15)	C21—C22—H22	120.8
N2—C6—N1	127.44 (14)	C23—C22—H22	120.8
N2—C6—C7	114.77 (13)	C24—C23—C22	120.19 (17)
N1—C6—C7	117.78 (13)	C24—C23—H23	119.9
C8—C7—C15	120.34 (14)	C22—C23—H23	119.9
C8—C7—C6	119.34 (14)	C23—C24—C25	119.13 (18)
C15—C7—C6	120.21 (13)	C23—C24—H24	120.4
C7—C8—C9	121.96 (14)	C25—C24—H24	120.4
C7—C8—C16	122.72 (14)	F2—C25—C20	118.59 (15)
C9—C8—C16	115.30 (13)	F2—C25—C24	117.79 (17)
O5—C9—N3	120.97 (15)	C20—C25—C24	123.62 (17)
O5—C9—C8	123.08 (16)	O3—C17'—C18'	101.3 (15)
N3—C9—C8	115.92 (14)	O3—C17'—H17C	111.5
N3—C10—C11	121.13 (15)	C18'—C17'—H17C	111.5
N3—C10—C15	119.65 (14)	O3—C17'—H17D	111.5
C11—C10—C15	119.20 (16)	C18'—C17'—H17D	111.5
C12—C11—C10	120.47 (18)	H17C—C17'—H17D	109.3
C12—C11—H11	119.8	C17'—C18'—H18D	109.5
C10—C11—H11	119.8	C17'—C18'—H18E	109.5
C11—C12—C13	120.80 (18)	H18D—C18'—H18E	109.5
C11—C12—H12	119.6	C17'—C18'—H18F	109.5
C13—C12—H12	119.6	H18D—C18'—H18F	109.5
C14—C13—C12	119.56 (19)	H18E—C18'—H18F	109.5
C14—C13—H13	120.2	C6—N1—C3	114.74 (13)

C12—C13—H13	120.2	C6—N2—C5	115.55 (13)
C13—C14—C15	121.40 (18)	C9—N3—C10	123.44 (13)
C13—C14—H14	119.3	C9—N3—C19	115.86 (14)
C15—C14—H14	119.3	C10—N3—C19	120.65 (14)
C14—C15—C10	118.57 (15)	C3—O1—C1	117.42 (13)
C14—C15—C7	123.14 (15)	C5—O2—C2	117.42 (14)
C10—C15—C7	118.26 (14)	C16—O3—C17'	131.7 (11)
O4—C16—O3	124.43 (16)	C16—O3—C17	112.5 (2)
O4—C16—C8	124.90 (15)		
N1—C3—C4—C5	0.5 (3)	F1—C21—C22—C23	−179.35 (17)
O1—C3—C4—C5	−179.25 (17)	C20—C21—C22—C23	0.2 (3)
C3—C4—C5—N2	−1.1 (3)	C21—C22—C23—C24	0.5 (3)
C3—C4—C5—O2	178.68 (17)	C22—C23—C24—C25	−0.7 (3)
N2—C6—C7—C8	−52.6 (2)	C21—C20—C25—F2	−179.00 (17)
N1—C6—C7—C8	126.78 (16)	C19—C20—C25—F2	4.1 (3)
N2—C6—C7—C15	123.54 (15)	C21—C20—C25—C24	0.6 (3)
N1—C6—C7—C15	−57.1 (2)	C19—C20—C25—C24	−176.27 (18)
C15—C7—C8—C9	−0.2 (2)	C23—C24—C25—F2	179.68 (17)
C6—C7—C8—C9	175.94 (13)	C23—C24—C25—C20	0.1 (3)
C15—C7—C8—C16	−178.53 (14)	N2—C6—N1—C3	−0.6 (2)
C6—C7—C8—C16	−2.4 (2)	C7—C6—N1—C3	−179.86 (14)
C7—C8—C9—O5	−176.33 (16)	O1—C3—N1—C6	−179.98 (15)
C16—C8—C9—O5	2.1 (2)	C4—C3—N1—C6	0.3 (3)
C7—C8—C9—N3	5.3 (2)	N1—C6—N2—C5	0.0 (2)
C16—C8—C9—N3	−176.22 (13)	C7—C6—N2—C5	179.33 (14)
N3—C10—C11—C12	178.11 (17)	O2—C5—N2—C6	−178.93 (16)
C15—C10—C11—C12	−0.3 (3)	C4—C5—N2—C6	0.9 (3)
C10—C11—C12—C13	−0.2 (3)	O5—C9—N3—C10	173.80 (15)
C11—C12—C13—C14	0.3 (3)	C8—C9—N3—C10	−7.8 (2)
C12—C13—C14—C15	0.0 (3)	O5—C9—N3—C19	−3.7 (2)
C13—C14—C15—C10	−0.5 (3)	C8—C9—N3—C19	174.74 (13)
C13—C14—C15—C7	−178.73 (18)	C11—C10—N3—C9	−173.30 (15)
N3—C10—C15—C14	−177.77 (15)	C15—C10—N3—C9	5.1 (2)
C11—C10—C15—C14	0.6 (2)	C11—C10—N3—C19	4.0 (2)
N3—C10—C15—C7	0.5 (2)	C15—C10—N3—C19	−177.59 (14)
C11—C10—C15—C7	178.93 (15)	C20—C19—N3—C9	100.99 (18)
C8—C7—C15—C14	175.40 (16)	C20—C19—N3—C10	−76.5 (2)
C6—C7—C15—C14	−0.7 (2)	N1—C3—O1—C1	3.5 (3)
C8—C7—C15—C10	−2.8 (2)	C4—C3—O1—C1	−176.73 (18)
C6—C7—C15—C10	−178.90 (13)	N2—C5—O2—C2	6.1 (3)
C7—C8—C16—O4	125.57 (19)	C4—C5—O2—C2	−173.71 (19)
C9—C8—C16—O4	−52.9 (2)	O4—C16—O3—C17'	15.6 (12)
C7—C8—C16—O3	−55.7 (2)	C8—C16—O3—C17'	−163.2 (12)
C9—C8—C16—O3	125.83 (15)	O4—C16—O3—C17	−8.7 (4)
N3—C19—C20—C25	−18.2 (3)	C8—C16—O3—C17	172.5 (3)
N3—C19—C20—C21	165.02 (16)	C18'—C17'—O3—C16	−108 (2)
C25—C20—C21—F1	178.84 (16)	C18'—C17'—O3—C17	−54 (2)
C19—C20—C21—F1	−4.0 (2)	C18—C17—O3—C16	−169.3 (7)
C25—C20—C21—C22	−0.8 (3)	C18—C17—O3—C17'	51.6 (15)

C19—C20—C21—C22	176.41 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19A···O5	0.97	2.25	2.665 (2)	105
C14—H14···N1	0.93	2.51	3.064 (2)	119
C23—H23···O4^{i}	0.93	2.52	3.288 (3)	140

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

Fig. 1

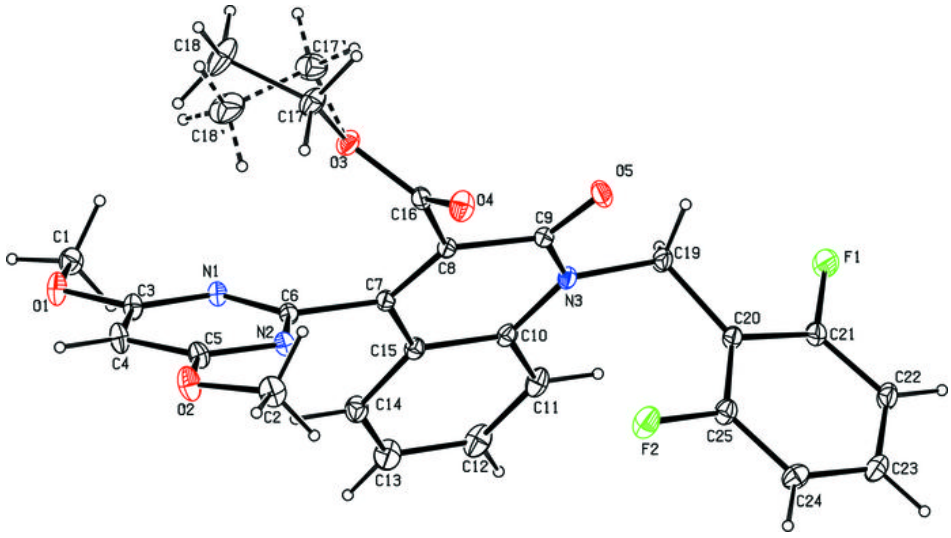
C18
C17'
C17
C18'
O3
O4
O5
C16
C9
C8
C1
O1
C3
N1
C6
C7
N3
C19
F1
C20
C21
C22
C5
N2
C15
C10
C4
O2
C2
C14
C11
F2
C25
C23
C13
C12
C24

Fig. 2