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2-{3-[2-(2,6-Difluorobenzyloxy)phenyl]-1*H*-pyrazol-1-yl}-4,6-dimethoxy-pyrimidine

Yuanxiang Li* and Chunping He

Chemistry and Chemical Engineering Department, Huaihua University, Huaihua 418008, People's Republic of China
Correspondence e-mail: hhhhxylyx@yahoo.com.cn

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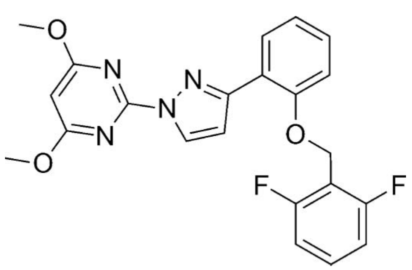
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.063; wR factor = 0.152; data-to-parameter ratio = 17.5.

In the title compound, $C_{22}H_{18}F_2N_4O_3$, the pyrimidine and pyrazole rings are nearly coplanar [dihedral angle = 2.93 (15)°]. The dihedral angle between the pyrazole ring and its attached benzene ring is 33.75 (3)°. Offset π–π stacking interactions involving the pyrimidine rings help to establish the packing [centroid–centroid separations = 3.7845 (17) and 3.9069 (17) Å].

Related literature

For background, see: Duggleby & Pang (2000). For a related structure, see: Li & Wang (2007). For reference geometrical data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{18}F_2N_4O_3$
M_r = 424.40
Orthorhombic, $Pccn$
a = 30.6872 (17) Å
b = 7.4261 (4) Å
c = 17.7703 (10) Å
V = 4049.6 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.35 × 0.20 × 0.08 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
37034 measured reflections
4949 independent reflections
2807 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.152
S = 1.04
4949 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2639).

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supplementary materials

Acta Cryst. (2007). E**63**, o4856 [**doi:10.1107/S1600536807060278**]

2-{3-[2-(2,6-Difluorobenzyloxy)phenyl]-1*H*-pyrazol-1-yl}-4,6-dimethoxypyrimidine

Y. Li and C. He

Comment

Pyrimidine derivatives have broad biological properties: in particular pyrimidinylbenzoate is a highly effective herbicide 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) and are in accordance with the corresponding values in similar compounds (Li & Wang, 2007). The pyrimidine ring A (N1,N2/C3–6) and pyrazole ring B (N3,N4/C7–9) in (I) are nearly coplanar with a dihedral angle of 2.93 (15)°. The dihedral angle between the pyrazole ring B (N3,N4/C7–9) and benzene ring C (C10—C15) is 33.75 (3)°. Benzene ring C (C10—C15) and benzene ring D (C17—C22) are nearly perpendicular with a dihedral angle of 86.74 (11)°.

Offset π-π stacking interactions involving the pyrimidine rings help to establish the packing. The adjacent rings have a centroid-centroid distance of 3.7845 (17)Å (symmetry: $1/2 - x$, $3/2 - y$, z) and 3.9069 (17)Å ($1/2 - x$, $5/2 - y$, z), leading to stacks propagating in [010].

Experimental

The title compound was synthesized according to the literature method (Li & Wang, 2007). Colourless plates of (I) were obtained by slow evaporation of a dichloromethane solution at 283 K.

Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Figures

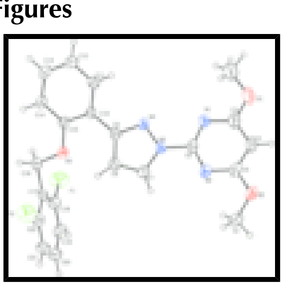

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms).

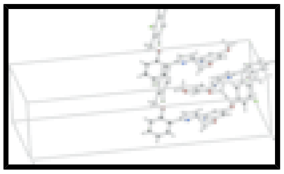
Fig. 2. A packing diagram for (I).

2-{3-[2-(2,6-Difluorobenzyloxy)phenyl]-1*H*-pyrazol-1-yl}-4,6-dimethoxypyrimidine

Crystal data

$C_{22}H_{18}F_2N_4O_3$	F_{000} = 1760
M_r = 424.40	D_x = 1.392 Mg m^{-3}
Orthorhombic, *Pccn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 3255 reflections
a = 30.6872 (17) Å	θ = 2.4–20.0°
b = 7.4261 (4) Å	μ = 0.11 mm^{-1}
c = 17.7703 (10) Å	*T* = 298 (2) K
V = 4049.6 (4) Å^3	Plate, colourless
Z = 8	0.35 × 0.20 × 0.08 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2807 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.074
Monochromator: graphite	θ_{max} = 28.3°
T = 298(2) K	θ_{min} = 1.3°
φ and ω scans	*h* = −40→40
Absorption correction: none	*k* = −9→9
37034 measured reflections	*l* = −23→23
4949 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
$R[F^2 > 2\sigma(F^2)]$ = 0.063	H-atom parameters constrained
$wR(F^2)$ = 0.152	$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 1.5034P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ < 0.001
4949 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
282 parameters	$\Delta\rho_{min}$ = −0.17 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}
C1	0.21023 (11)	1.0322 (9)	−0.24781 (19)	0.165 (3)
H1A	0.1929	0.9303	−0.2334	0.248*
H1B	0.2106	1.0421	−0.3017	0.248*
H1C	0.1979	1.1397	−0.2266	0.248*
C2	0.35015 (9)	0.9178 (4)	0.06488 (17)	0.0748 (8)
H2A	0.3425	1.0316	0.0868	0.112*
H2B	0.3799	0.8902	0.0766	0.112*
H2C	0.3316	0.8254	0.0848	0.112*
C3	0.25983 (9)	1.0031 (5)	−0.14530 (16)	0.0826 (10)
C4	0.30104 (8)	0.9710 (5)	−0.11906 (16)	0.0784 (9)
H4	0.3246	0.9554	−0.1512	0.094*
C5	0.30535 (7)	0.9635 (4)	−0.04237 (15)	0.0572 (7)
C6	0.23425 (7)	1.0204 (3)	−0.02895 (14)	0.0481 (6)
N1	0.22532 (6)	1.0283 (3)	−0.10123 (12)	0.0657 (6)
C7	0.19998 (7)	1.0348 (4)	0.09684 (13)	0.0556 (7)
H7	0.2243	1.0116	0.1265	0.067*
C8	0.15884 (7)	1.0629 (4)	0.12144 (13)	0.0563 (7)
H8	0.1491	1.0619	0.1710	0.068*
C9	0.13382 (7)	1.0942 (3)	0.05642 (12)	0.0413 (5)
C10	0.08717 (7)	1.1413 (3)	0.04837 (12)	0.0405 (5)
C11	0.07378 (7)	1.2571 (3)	−0.00832 (12)	0.0479 (6)
H11	0.0945	1.3054	−0.0408	0.057*
C12	0.03068 (8)	1.3026 (3)	−0.01790 (14)	0.0538 (6)
H12	0.0224	1.3790	−0.0568	0.065*
C13	−0.00004 (7)	1.2338 (3)	0.03074 (14)	0.0550 (6)
H13	−0.0292	1.2646	0.0247	0.066*
C14	0.01201 (7)	1.1197 (3)	0.08842 (14)	0.0496 (6)
H14	−0.0088	1.0749	0.1215	0.060*
C15	0.05535 (7)	1.0726 (3)	0.09667 (12)	0.0432 (5)
C16	0.03880 (7)	0.8740 (4)	0.19954 (14)	0.0545 (7)
H16A	0.0156	0.8202	0.1702	0.065*
H16B	0.0262	0.9633	0.2330	0.065*
C17	0.06215 (6)	0.7331 (3)	0.24380 (12)	0.0465 (6)

C18	0.06393 (8)	0.5559 (4)	0.22116 (14)	0.0559 (7)
C19	0.08517 (9)	0.4232 (4)	0.25980 (17)	0.0691 (8)
H19	0.0854	0.3052	0.2423	0.083*
C20	0.10615 (8)	0.4699 (5)	0.32536 (17)	0.0729 (9)
H20	0.1209	0.3819	0.3526	0.087*
C21	0.10569 (8)	0.6437 (5)	0.35129 (15)	0.0700 (8)
H21	0.1197	0.6747	0.3959	0.084*
C22	0.08414 (8)	0.7694 (4)	0.30994 (14)	0.0575 (7)
F1	0.04302 (6)	0.5126 (2)	0.15660 (9)	0.0885 (6)
F2	0.08362 (6)	0.9420 (3)	0.33448 (10)	0.0943 (6)
N4	0.15827 (5)	1.0841 (3)	−0.00498 (10)	0.0439 (5)
N3	0.19907 (5)	1.0467 (3)	0.02097 (10)	0.0446 (5)
N2	0.27208 (6)	0.9881 (3)	0.00467 (11)	0.0498 (5)
O1	0.25419 (7)	1.0092 (5)	−0.22035 (11)	0.1358 (13)
O2	0.34493 (5)	0.9270 (3)	−0.01474 (11)	0.0682 (5)
O3	0.07009 (5)	0.9556 (2)	0.15119 (9)	0.0580 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.061 (2)	0.376 (8)	0.059 (2)	0.024 (3)	−0.0031 (17)	0.005 (3)
C2	0.0513 (15)	0.084 (2)	0.089 (2)	0.0069 (15)	−0.0063 (14)	0.0126 (17)
C3	0.0498 (16)	0.142 (3)	0.0562 (17)	0.0082 (17)	0.0094 (13)	−0.0038 (18)
C4	0.0448 (15)	0.124 (3)	0.0662 (19)	0.0101 (16)	0.0158 (13)	−0.0080 (18)
C5	0.0367 (12)	0.0624 (17)	0.0726 (18)	0.0046 (12)	0.0043 (12)	−0.0043 (14)
C6	0.0366 (12)	0.0525 (15)	0.0552 (15)	−0.0027 (11)	0.0071 (10)	−0.0009 (12)
N1	0.0411 (11)	0.107 (2)	0.0488 (13)	0.0050 (12)	0.0050 (9)	0.0010 (12)
C7	0.0423 (13)	0.0790 (19)	0.0455 (14)	−0.0006 (12)	−0.0066 (10)	−0.0010 (13)
C8	0.0416 (13)	0.087 (2)	0.0401 (13)	−0.0008 (13)	0.0010 (10)	−0.0021 (13)
C9	0.0375 (11)	0.0434 (14)	0.0428 (12)	−0.0018 (10)	0.0017 (10)	−0.0021 (10)
C10	0.0369 (11)	0.0440 (13)	0.0405 (12)	0.0022 (10)	0.0003 (9)	−0.0070 (10)
C11	0.0474 (13)	0.0510 (15)	0.0452 (13)	0.0006 (11)	0.0000 (10)	−0.0030 (11)
C12	0.0557 (14)	0.0509 (16)	0.0546 (15)	0.0093 (12)	−0.0123 (12)	−0.0008 (12)
C13	0.0409 (12)	0.0569 (16)	0.0672 (16)	0.0112 (12)	−0.0079 (12)	−0.0096 (13)
C14	0.0366 (12)	0.0549 (16)	0.0573 (14)	0.0045 (11)	0.0027 (10)	−0.0059 (12)
C15	0.0407 (12)	0.0443 (14)	0.0446 (12)	0.0054 (10)	0.0004 (10)	−0.0029 (11)
C16	0.0379 (12)	0.0705 (18)	0.0550 (15)	0.0000 (12)	0.0075 (11)	0.0057 (13)
C17	0.0348 (11)	0.0630 (17)	0.0416 (12)	−0.0061 (11)	0.0057 (9)	0.0055 (12)
C18	0.0460 (14)	0.073 (2)	0.0490 (14)	−0.0054 (13)	−0.0027 (11)	−0.0015 (13)
C19	0.0632 (17)	0.0643 (19)	0.080 (2)	0.0032 (14)	0.0038 (15)	0.0079 (16)
C20	0.0495 (15)	0.096 (3)	0.073 (2)	0.0051 (16)	0.0006 (14)	0.0332 (19)
C21	0.0552 (16)	0.102 (3)	0.0525 (16)	−0.0154 (16)	−0.0110 (13)	0.0122 (17)
C22	0.0497 (13)	0.0699 (19)	0.0528 (15)	−0.0138 (13)	0.0016 (12)	−0.0034 (14)
F1	0.0992 (13)	0.0920 (13)	0.0741 (11)	0.0054 (10)	−0.0285 (9)	−0.0261 (10)
F2	0.1061 (14)	0.0863 (14)	0.0906 (13)	−0.0140 (10)	−0.0164 (10)	−0.0257 (10)
N4	0.0342 (9)	0.0539 (12)	0.0437 (11)	0.0023 (8)	0.0000 (8)	−0.0013 (9)
N3	0.0330 (9)	0.0564 (13)	0.0442 (11)	−0.0013 (9)	0.0010 (8)	−0.0019 (9)
N2	0.0365 (10)	0.0533 (13)	0.0596 (12)	−0.0021 (9)	0.0028 (9)	−0.0007 (10)

O1	0.0575 (13)	0.295 (4)	0.0543 (12)	0.0217 (18)	0.0104 (10)	−0.0055 (18)
O2	0.0393 (9)	0.0869 (14)	0.0783 (13)	0.0109 (9)	0.0007 (9)	−0.0030 (11)
O3	0.0346 (8)	0.0759 (12)	0.0634 (11)	0.0051 (8)	0.0073 (7)	0.0230 (9)

Geometric parameters (Å, °)

C1—O1	1.445 (4)	C10—C15	1.397 (3)
C1—H1A	0.9600	C11—C12	1.376 (3)
C1—H1B	0.9600	C11—H11	0.9300
C1—H1C	0.9600	C12—C13	1.377 (3)
C2—O2	1.426 (3)	C12—H12	0.9300
C2—H2A	0.9600	C13—C14	1.380 (3)
C2—H2B	0.9600	C13—H13	0.9300
C2—H2C	0.9600	C14—C15	1.383 (3)
C3—N1	1.330 (3)	C14—H14	0.9300
C3—O1	1.346 (3)	C15—O3	1.378 (3)
C3—C4	1.369 (4)	C16—O3	1.424 (3)
C4—C5	1.370 (4)	C16—C17	1.493 (3)
C4—H4	0.9300	C16—H16A	0.9700
C5—N2	1.332 (3)	C16—H16B	0.9700
C5—O2	1.338 (3)	C17—C18	1.377 (4)
C6—N1	1.315 (3)	C17—C22	1.382 (3)
C6—N2	1.327 (3)	C18—F1	1.353 (3)
C6—N3	1.411 (3)	C18—C19	1.367 (4)
C7—N3	1.351 (3)	C19—C20	1.375 (4)
C7—C8	1.352 (3)	C19—H19	0.9300
C7—H7	0.9300	C20—C21	1.371 (4)
C8—C9	1.407 (3)	C20—H20	0.9300
C8—H8	0.9300	C21—C22	1.360 (4)
C9—N4	1.326 (3)	C21—H21	0.9300
C9—C10	1.480 (3)	C22—F2	1.354 (3)
C10—C11	1.387 (3)	N4—N3	1.363 (2)
O1—C1—H1A	109.5	C13—C12—H12	120.3
O1—C1—H1B	109.5	C12—C13—C14	120.7 (2)
H1A—C1—H1B	109.5	C12—C13—H13	119.7
O1—C1—H1C	109.5	C14—C13—H13	119.7
H1A—C1—H1C	109.5	C13—C14—C15	119.4 (2)
H1B—C1—H1C	109.5	C13—C14—H14	120.3
O2—C2—H2A	109.5	C15—C14—H14	120.3
O2—C2—H2B	109.5	O3—C15—C14	123.4 (2)
H2A—C2—H2B	109.5	O3—C15—C10	115.66 (18)
O2—C2—H2C	109.5	C14—C15—C10	121.0 (2)
H2A—C2—H2C	109.5	O3—C16—C17	107.02 (17)
H2B—C2—H2C	109.5	O3—C16—H16A	110.3
N1—C3—O1	118.5 (2)	C17—C16—H16A	110.3
N1—C3—C4	124.0 (3)	O3—C16—H16B	110.3
O1—C3—C4	117.5 (2)	C17—C16—H16B	110.3
C3—C4—C5	115.8 (2)	H16A—C16—H16B	108.6
C3—C4—H4	122.1	C18—C17—C22	114.6 (2)

C5—C4—H4	122.1	C18—C17—C16	122.4 (2)
N2—C5—O2	119.6 (2)	C22—C17—C16	123.1 (2)
N2—C5—C4	123.0 (2)	F1—C18—C19	118.7 (3)
O2—C5—C4	117.5 (2)	F1—C18—C17	117.1 (2)
N1—C6—N2	129.1 (2)	C19—C18—C17	124.1 (2)
N1—C6—N3	116.7 (2)	C18—C19—C20	117.9 (3)
N2—C6—N3	114.3 (2)	C18—C19—H19	121.1
C6—N1—C3	113.8 (2)	C20—C19—H19	121.1
N3—C7—C8	107.0 (2)	C21—C20—C19	121.1 (3)
N3—C7—H7	126.5	C21—C20—H20	119.4
C8—C7—H7	126.5	C19—C20—H20	119.4
C7—C8—C9	105.6 (2)	C22—C21—C20	118.0 (3)
C7—C8—H8	127.2	C22—C21—H21	121.0
C9—C8—H8	127.2	C20—C21—H21	121.0
N4—C9—C8	110.95 (18)	F2—C22—C21	118.8 (3)
N4—C9—C10	118.74 (19)	F2—C22—C17	116.9 (2)
C8—C9—C10	130.3 (2)	C21—C22—C17	124.3 (3)
C11—C10—C15	117.77 (19)	C9—N4—N3	104.65 (17)
C11—C10—C9	120.2 (2)	C7—N3—N4	111.71 (17)
C15—C10—C9	122.0 (2)	C7—N3—C6	127.03 (19)
C12—C11—C10	121.8 (2)	N4—N3—C6	121.23 (18)
C12—C11—H11	119.1	C6—N2—C5	114.4 (2)
C10—C11—H11	119.1	C3—O1—C1	117.3 (2)
C11—C12—C13	119.3 (2)	C5—O2—C2	118.4 (2)
C11—C12—H12	120.3	C15—O3—C16	118.11 (16)

N1—C3—C4—C5	0.8 (5)	F1—C18—C19—C20	−179.9 (2)
O1—C3—C4—C5	−179.2 (3)	C17—C18—C19—C20	−0.1 (4)
C3—C4—C5—N2	−1.0 (5)	C18—C19—C20—C21	0.2 (4)
C3—C4—C5—O2	178.0 (3)	C19—C20—C21—C22	−0.5 (4)
N2—C6—N1—C3	−1.4 (4)	C20—C21—C22—F2	−179.5 (2)
N3—C6—N1—C3	179.8 (3)	C20—C21—C22—C17	0.8 (4)
O1—C3—N1—C6	−179.8 (3)	C18—C17—C22—F2	179.6 (2)
C4—C3—N1—C6	0.3 (5)	C16—C17—C22—F2	0.5 (3)
N3—C7—C8—C9	−0.7 (3)	C18—C17—C22—C21	−0.8 (3)
C7—C8—C9—N4	0.5 (3)	C16—C17—C22—C21	−179.9 (2)
C7—C8—C9—C10	−176.7 (2)	C8—C9—N4—N3	−0.1 (3)
N4—C9—C10—C11	−32.8 (3)	C10—C9—N4—N3	177.48 (19)
C8—C9—C10—C11	144.3 (3)	C8—C7—N3—N4	0.7 (3)
N4—C9—C10—C15	147.3 (2)	C8—C7—N3—C6	−177.6 (2)
C8—C9—C10—C15	−35.6 (4)	C9—N4—N3—C7	−0.3 (3)
C15—C10—C11—C12	−0.7 (3)	C9—N4—N3—C6	178.0 (2)
C9—C10—C11—C12	179.4 (2)	N1—C6—N3—C7	176.1 (2)
C10—C11—C12—C13	1.0 (4)	N2—C6—N3—C7	−3.0 (3)
C11—C12—C13—C14	−0.3 (4)	N1—C6—N3—N4	−2.0 (3)
C12—C13—C14—C15	−0.8 (4)	N2—C6—N3—N4	178.9 (2)
C13—C14—C15—O3	−178.1 (2)	N1—C6—N2—C5	1.2 (4)
C13—C14—C15—C10	1.2 (3)	N3—C6—N2—C5	−179.9 (2)
C11—C10—C15—O3	178.9 (2)	O2—C5—N2—C6	−178.9 (2)
C9—C10—C15—O3	−1.2 (3)	C4—C5—N2—C6	0.1 (4)

C11—C10—C15—C14	−0.5 (3)	N1—C3—O1—C1	−3.6 (6)
C9—C10—C15—C14	179.5 (2)	C4—C3—O1—C1	176.4 (4)
O3—C16—C17—C18	−93.3 (3)	N2—C5—O2—C2	−0.7 (4)
O3—C16—C17—C22	85.8 (3)	C4—C5—O2—C2	−179.8 (3)
C22—C17—C18—F1	−179.9 (2)	C14—C15—O3—C16	2.5 (3)
C16—C17—C18—F1	−0.7 (3)	C10—C15—O3—C16	−176.8 (2)
C22—C17—C18—C19	0.4 (3)	C17—C16—O3—C15	170.8 (2)
C16—C17—C18—C19	179.6 (2)		

Fig. 1

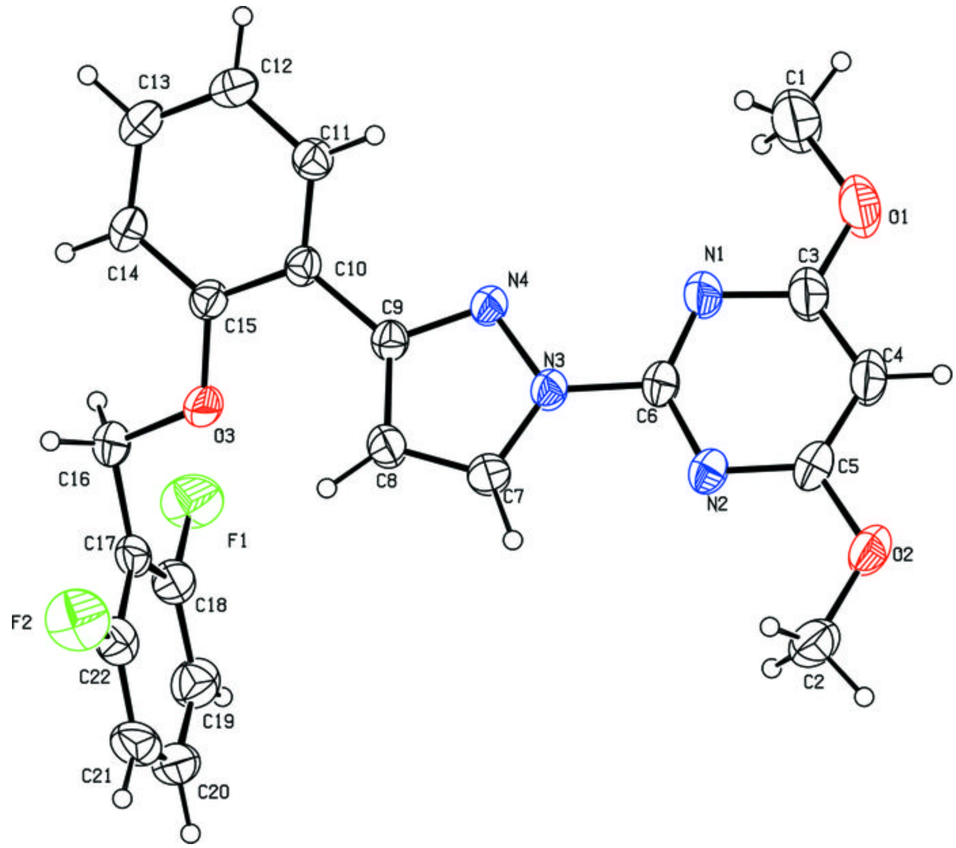
C1
O1
C3
N1
C4
C5
N2
C6
O2
C2
N3
N4
C9
C10
C11
C12
C13
C14
C15
O3
C16
C17
C18
F1
F2
C22
C19
C21
C20
C8
C7

Fig. 2