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(*R*)-Prop-2-ynyl 2-[4-(5-chloro-3-fluoropyridin-2-yloxy)phenoxy]propanoate

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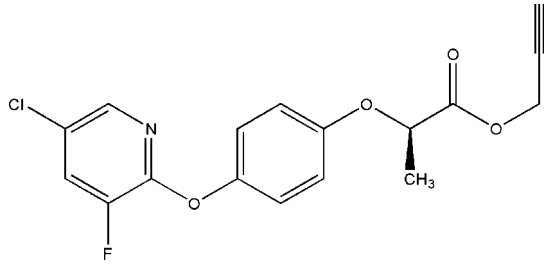
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.060; wR factor = 0.170; data-to-parameter ratio = 8.2.

The asymmetric unit of the title compound, $C_{17}H_{13}ClFNO_4$, contains two independent molecules. The dihedral angles between the pyridine and benzene rings are 83.3 (2) and 69.7 (1)° in the two molecules. In the crystal structure, intermolecular C—H···N and C—H···F hydrogen bonds link the molecules into chains.

Related literature

For general background, see: Chen *et al.* (2005); Allen *et al.* (1987). For related literature, see: Chen *et al.* (2005).



Experimental

Crystal data

$C_{17}H_{13}ClFNO_4$
M_r = 349.73
Monoclinic, $C2$
a = 37.867 (3) Å
b = 8.1682 (11) Å
c = 10.9666 (14) Å
β = 93.45 (3)°
V = 3385.8 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 298 (2) K
0.40 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.905, T_{max} = 0.975
3550 measured reflections
3550 independent reflections
2149 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.170
S = 1.01
3550 reflections
433 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), with 57 Friedel pairs
Flack parameter: 0.28 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···F1^{i}	0.98	2.47	3.433 (9)	169
C20—H20A···N1^{ii}	0.97	2.58	3.554 (9)	179

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: HK2242).

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supplementary materials

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(*R*)-Prop-2-ynyl 2-[4-(5-chloro-3-fluoropyridin-2-yloxy)phenoxy]propanoate

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Comment

The title compound, (I), can be used as an important herbicide (Chen *et al.*, 2005). We herein report its crystal structure.

The asymmetric unit of the title compound, (I), (Fig. 1), contains two independent molecules and the bond lengths and angles (Table 1) are generally within normal ranges (Allen *et al.*, 1987).

Rings A (C7—C12), B (N1/C13—C17), C (C24—C29) and D (N2/C30—C34) are, of course, planar and the dihedral angles between them are A/B = 83.3 (2)° and C/D = 69.7 (1)°.

As can be seen from the packing diagram (Fig. 2), the intermolecular C—H···N and C—H···F hydrogen bonds (Table 2) link the molecules into chains, in which they may be effective in the stabilization of the crystal structure. Dipol-dipol and van der Waals interactions are also effective in the molecular packing.

Experimental

The title compound, (I) was prepared by the literature method (Chen *et al.*, 2005). The crystals were obtained by dissolving the title compound (0.5 g) in ethanol (50 ml) and evaporating the solvent slowly at room temperature for about 20 d.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 (for aromatic H), 0.96 and 0.98 (for methine H), 0.97 (for methylene H) and 0.96 Å (for methyl H), and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

Figures

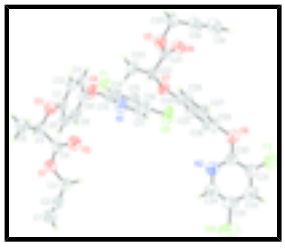

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

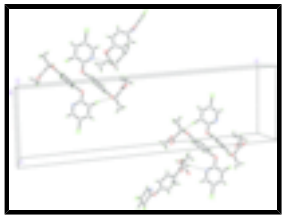

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

(*R*)-Prop-2-ynyl 2-(4-(5-chloro-3-fluoropyridin-2-yloxy)phenoxy)propanoate

Crystal data

$C_{17}H_{13}ClFNO_4$	F_{000} = 1440
M_r = 349.73	D_x = 1.372 Mg m^{-3}
Monoclinic, *C*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2y	Cell parameters from 25 reflections
a = 37.867 (3) Å	θ = 10–13º
b = 8.1682 (11) Å	μ = 0.26 mm^{-1}
c = 10.9666 (14) Å	*T* = 298 (2) K
β = 93.45 (3)º	Block, colourless
V = 3385.8 (7) Å^3	0.40 × 0.30 × 0.10 mm
Z = 8	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.0000
Radiation source: fine-focus sealed tube	θ_{max} = 26.0º
Monochromator: graphite	θ_{min} = 1.9º
T = 298(2) K	*h* = −46→46
ω/2θ scans	*k* = 0→10
Absorption correction: ψ scan (North *et al.*, 1968)	*l* = 0→13
T_{min} = 0.905, T_{max} = 0.975	3 standard reflections
3550 measured reflections	every 200 reflections
3550 independent reflections	intensity decay: none
2149 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.060	$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.170	$(\Delta/\sigma)_{max} < 0.001$
S = 1.01	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
3550 reflections	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
433 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 57 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.28 (17)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
Cl1	0.73191 (7)	0.0546 (6)	0.65536 (19)	0.1523 (13)
F1	0.80852 (10)	0.0049 (9)	0.2946 (4)	0.128 (2)
O1	0.59918 (12)	−0.4128 (5)	−0.1417 (4)	0.0795 (13)
O2	0.58657 (14)	−0.1584 (7)	−0.0911 (5)	0.0910 (14)
O3	0.64375 (11)	−0.0513 (5)	−0.2150 (4)	0.0740 (12)
O4	0.75258 (11)	0.0099 (9)	0.1393 (4)	0.0987 (18)
C1	0.5857 (2)	−0.7883 (10)	−0.0409 (7)	0.094 (2)
H1B	0.5821	−0.8706	0.0196	0.113*
C2	0.57952 (18)	−0.6421 (9)	−0.0437 (6)	0.0756 (18)
C3	0.57404 (18)	−0.4697 (9)	−0.0569 (6)	0.0770 (18)
H3A	0.5780	−0.4152	0.0214	0.092*
H3B	0.5500	−0.4473	−0.0884	0.092*
C4	0.60275 (17)	−0.2506 (8)	−0.1507 (5)	0.0661 (16)
C5	0.62827 (18)	−0.2057 (8)	−0.2441 (5)	0.0696 (16)
H5A	0.6467	−0.2895	−0.2468	0.084*
C6	0.6092 (2)	−0.1865 (11)	−0.3709 (6)	0.097 (2)
H6A	0.6261	−0.1585	−0.4293	0.146*
H6B	0.5918	−0.1013	−0.3683	0.146*
H6C	0.5978	−0.2877	−0.3943	0.146*
C7	0.66962 (16)	−0.0437 (8)	−0.1219 (5)	0.0677 (15)
C8	0.68113 (16)	−0.1778 (9)	−0.0530 (5)	0.0744 (16)
H8A	0.6709	−0.2803	−0.0663	0.089*
C9	0.70829 (17)	−0.1555 (10)	0.0365 (6)	0.0807 (18)
H9A	0.7168	−0.2446	0.0823	0.097*
C10	0.72253 (16)	−0.0047 (10)	0.0578 (6)	0.0750 (17)
C11	0.71068 (18)	0.1297 (10)	−0.0103 (6)	0.0777 (17)
H11A	0.7207	0.2323	0.0035	0.093*
C12	0.68367 (16)	0.1082 (8)	−0.0991 (5)	0.0691 (15)
H12A	0.6749	0.1978	−0.1437	0.083*
C13	0.74679 (18)	0.0236 (10)	0.2593 (6)	0.0795 (17)
C14	0.77636 (18)	0.0194 (11)	0.3391 (7)	0.0830 (19)
C15	0.7726 (2)	0.0291 (14)	0.4631 (7)	0.106 (2)
H15A	0.7922	0.0250	0.5184	0.127*

C16	0.73960 (19)	0.0449 (13)	0.5018 (7)	0.093 (2)
C17	0.7112 (2)	0.0383 (12)	0.4175 (6)	0.098 (2)
H17A	0.6884	0.0398	0.4452	0.118*
N1	0.71505 (14)	0.0298 (10)	0.2976 (5)	0.0896 (17)
Cl2	0.48191 (7)	−0.2837 (4)	0.8097 (3)	0.1412 (11)
F2	0.49168 (14)	0.3296 (7)	0.8523 (4)	0.1204 (17)
O5	0.62661 (11)	0.7285 (6)	0.1873 (4)	0.0733 (11)
O6	0.65936 (12)	0.7104 (6)	0.3643 (4)	0.0802 (12)
O7	0.64525 (11)	0.3785 (6)	0.3673 (4)	0.0737 (12)
O8	0.53381 (13)	0.3496 (6)	0.6671 (4)	0.0879 (14)
C18	0.5838 (2)	1.0156 (11)	0.3580 (7)	0.095 (2)
H18A	0.5783	1.0352	0.4410	0.114*
C19	0.60420 (19)	0.9631 (9)	0.2865 (6)	0.0768 (18)
C20	0.6280 (2)	0.9058 (8)	0.1992 (6)	0.0787 (19)
H20A	0.6519	0.9389	0.2246	0.094*
H20B	0.6219	0.9555	0.1205	0.094*
C21	0.64394 (16)	0.6436 (8)	0.2784 (6)	0.0631 (15)
C22	0.64261 (18)	0.4643 (8)	0.2552 (5)	0.0684 (16)
H22A	0.6204	0.4360	0.2098	0.082*
C23	0.6734 (2)	0.4140 (10)	0.1834 (6)	0.098 (2)
H23A	0.6723	0.4709	0.1066	0.147*
H23B	0.6724	0.2981	0.1690	0.147*
H23C	0.6951	0.4409	0.2287	0.147*
C24	0.61667 (15)	0.3803 (8)	0.4379 (5)	0.0608 (13)
C25	0.62184 (17)	0.3046 (8)	0.5506 (5)	0.0695 (15)
H25A	0.6439	0.2621	0.5750	0.083*
C26	0.59456 (18)	0.2923 (9)	0.6255 (6)	0.0727 (16)
H26A	0.5981	0.2424	0.7015	0.087*
C27	0.55670 (16)	0.4337 (8)	0.4797 (6)	0.0700 (15)
H27A	0.5348	0.4789	0.4568	0.084*
C28	0.58474 (17)	0.4471 (8)	0.4028 (6)	0.0727 (16)
H28A	0.5816	0.5012	0.3283	0.087*
C29	0.56190 (17)	0.3531 (8)	0.5894 (5)	0.0714 (16)
C30	0.52142 (16)	0.2002 (9)	0.6994 (6)	0.0710 (15)
C31	0.49999 (18)	0.1923 (10)	0.7938 (7)	0.0802 (18)
C32	0.48724 (19)	0.0456 (12)	0.8321 (6)	0.091 (2)
H32A	0.4730	0.0389	0.8980	0.109*
C33	0.49657 (19)	−0.0919 (10)	0.7685 (8)	0.089 (2)
C34	0.5168 (2)	−0.0765 (10)	0.6734 (8)	0.089 (2)
H34A	0.5223	−0.1701	0.6301	0.107*
N2	0.52953 (15)	0.0690 (8)	0.6374 (5)	0.0831 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.146 (2)	0.243 (4)	0.0682 (11)	−0.002 (3)	0.0094 (12)	−0.027 (2)
F1	0.067 (2)	0.213 (6)	0.103 (3)	−0.017 (3)	−0.007 (2)	0.012 (4)
O1	0.107 (3)	0.055 (3)	0.077 (3)	−0.008 (2)	0.019 (2)	−0.008 (2)

O2	0.103 (4)	0.082 (3)	0.090 (3)	0.005 (3)	0.016 (3)	−0.004 (3)
O3	0.088 (3)	0.068 (3)	0.065 (2)	−0.008 (2)	−0.007 (2)	0.004 (2)
O4	0.064 (2)	0.163 (5)	0.068 (3)	−0.023 (3)	0.005 (2)	0.000 (3)
C1	0.114 (6)	0.082 (6)	0.085 (5)	−0.007 (5)	0.000 (4)	0.017 (4)
C2	0.084 (4)	0.085 (5)	0.058 (4)	0.001 (4)	0.001 (3)	0.005 (3)
C3	0.087 (4)	0.069 (4)	0.076 (4)	−0.008 (4)	0.017 (3)	−0.003 (4)
C4	0.079 (4)	0.062 (4)	0.057 (3)	0.008 (3)	0.000 (3)	−0.014 (3)
C5	0.091 (4)	0.061 (4)	0.056 (3)	−0.002 (3)	−0.002 (3)	−0.008 (3)
C6	0.126 (6)	0.109 (6)	0.056 (4)	−0.019 (5)	−0.002 (4)	−0.011 (4)
C7	0.069 (3)	0.075 (4)	0.059 (3)	−0.006 (3)	0.001 (3)	−0.001 (3)
C8	0.073 (4)	0.080 (4)	0.069 (3)	−0.008 (3)	0.000 (3)	0.006 (3)
C9	0.071 (4)	0.101 (4)	0.070 (4)	−0.004 (4)	0.002 (3)	0.018 (4)
C10	0.062 (3)	0.106 (5)	0.058 (3)	0.000 (3)	0.007 (3)	−0.008 (3)
C11	0.081 (4)	0.085 (4)	0.068 (4)	−0.014 (3)	0.013 (3)	−0.013 (3)
C12	0.080 (4)	0.074 (4)	0.055 (3)	0.002 (3)	0.013 (3)	−0.004 (3)
C13	0.078 (4)	0.096 (5)	0.065 (3)	−0.015 (4)	0.003 (3)	−0.010 (4)
C14	0.068 (3)	0.097 (5)	0.085 (4)	−0.014 (4)	0.007 (3)	0.002 (4)
C15	0.104 (4)	0.135 (6)	0.077 (4)	−0.001 (5)	−0.005 (4)	−0.002 (5)
C16	0.092 (4)	0.112 (5)	0.077 (4)	−0.007 (4)	0.010 (3)	−0.011 (4)
C17	0.090 (4)	0.128 (6)	0.077 (4)	0.001 (5)	0.010 (3)	−0.015 (5)
N1	0.075 (3)	0.121 (5)	0.073 (3)	0.007 (3)	0.007 (3)	−0.014 (4)
Cl2	0.1080 (16)	0.125 (2)	0.187 (3)	−0.0316 (16)	−0.0179 (16)	0.059 (2)
F2	0.127 (4)	0.129 (4)	0.111 (3)	−0.026 (3)	0.051 (3)	−0.030 (3)
O5	0.087 (3)	0.077 (3)	0.054 (2)	0.009 (2)	−0.008 (2)	−0.003 (2)
O6	0.093 (3)	0.072 (3)	0.072 (3)	0.001 (3)	−0.020 (2)	0.000 (2)
O7	0.085 (3)	0.077 (3)	0.060 (2)	0.016 (2)	0.015 (2)	0.014 (2)
O8	0.089 (3)	0.091 (4)	0.086 (3)	−0.005 (3)	0.026 (2)	−0.002 (3)
C18	0.106 (6)	0.092 (6)	0.084 (5)	0.010 (5)	−0.026 (4)	−0.016 (4)
C19	0.098 (5)	0.063 (4)	0.066 (4)	0.000 (4)	−0.026 (4)	−0.008 (3)
C20	0.118 (5)	0.063 (4)	0.054 (4)	0.004 (4)	−0.003 (4)	0.007 (3)
C21	0.068 (4)	0.068 (4)	0.054 (3)	0.010 (3)	0.008 (3)	0.010 (3)
C22	0.087 (4)	0.069 (4)	0.049 (3)	0.006 (3)	0.006 (3)	0.002 (3)
C23	0.132 (6)	0.095 (6)	0.070 (4)	0.031 (5)	0.042 (4)	0.013 (4)
C24	0.068 (3)	0.062 (3)	0.053 (3)	−0.003 (3)	0.003 (2)	0.001 (3)
C25	0.082 (4)	0.070 (4)	0.056 (3)	0.000 (3)	0.001 (3)	0.003 (3)
C26	0.089 (4)	0.080 (4)	0.050 (3)	−0.007 (3)	0.006 (3)	0.001 (3)
C27	0.066 (3)	0.068 (4)	0.075 (3)	−0.001 (3)	0.001 (3)	0.000 (3)
C28	0.081 (4)	0.070 (4)	0.066 (3)	−0.002 (3)	−0.001 (3)	0.007 (3)
C29	0.084 (4)	0.070 (4)	0.061 (3)	−0.005 (3)	0.013 (3)	−0.004 (3)
C30	0.070 (3)	0.078 (4)	0.065 (3)	−0.003 (3)	0.007 (3)	0.001 (3)
C31	0.074 (4)	0.095 (4)	0.072 (4)	−0.003 (4)	0.009 (3)	−0.009 (4)
C32	0.077 (4)	0.120 (5)	0.075 (4)	−0.018 (4)	0.005 (3)	0.011 (4)
C33	0.068 (4)	0.093 (4)	0.105 (5)	−0.017 (4)	−0.009 (3)	0.019 (4)
C34	0.085 (4)	0.073 (4)	0.110 (5)	−0.008 (4)	0.000 (4)	0.000 (4)
N2	0.085 (3)	0.083 (4)	0.083 (3)	−0.010 (3)	0.011 (3)	−0.002 (3)

Geometric parameters (Å, °)

Cl1—C16	1.728 (7)	Cl2—C33	1.731 (8)

F1—C14	1.344 (7)	F2—C31	1.339 (9)
O1—C4	1.337 (8)	O5—C21	1.353 (7)
O1—C3	1.447 (7)	O5—C20	1.455 (8)
O2—C4	1.191 (7)	O6—C21	1.208 (7)
O3—C7	1.373 (7)	O7—C24	1.368 (7)
O3—C5	1.419 (8)	O7—C22	1.414 (7)
O4—C13	1.352 (7)	O8—C30	1.362 (8)
O4—C10	1.409 (7)	O8—C29	1.402 (7)
C1—C2	1.216 (8)	C18—C19	1.211 (7)
C1—H1B	0.9600	C18—H18A	0.9599
C2—C3	1.430 (11)	C19—C20	1.432 (10)
C3—H3A	0.9700	C20—H20A	0.9700
C3—H3B	0.9700	C20—H20B	0.9700
C4—C5	1.496 (9)	C21—C22	1.487 (9)
C5—C6	1.535 (9)	C22—C23	1.502 (9)
C5—H5A	0.9800	C22—H22A	0.9800
C6—H6A	0.9600	C23—H23A	0.9600
C6—H6B	0.9600	C23—H23B	0.9600
C6—H6C	0.9600	C23—H23C	0.9600
C7—C12	1.367 (9)	C24—C28	1.361 (8)
C7—C8	1.386 (9)	C24—C25	1.385 (8)
C8—C9	1.390 (9)	C25—C26	1.362 (8)
C8—H8A	0.9300	C25—H25A	0.9300
C9—C10	1.359 (10)	C26—C29	1.369 (9)
C9—H9A	0.9300	C26—H26A	0.9300
C10—C11	1.387 (10)	C27—C29	1.376 (9)
C11—C12	1.380 (9)	C27—C28	1.399 (9)
C11—H11A	0.9300	C27—H27A	0.9300
C12—H12A	0.9300	C28—H28A	0.9300
C13—N1	1.298 (8)	C30—N2	1.315 (9)
C13—C14	1.379 (9)	C30—C31	1.354 (9)
C14—C15	1.378 (10)	C31—C32	1.368 (11)
C15—C16	1.352 (10)	C32—C33	1.380 (12)
C15—H15A	0.9300	C32—H32A	0.9300
C16—C17	1.377 (10)	C33—C34	1.335 (11)
C17—N1	1.334 (8)	C34—N2	1.351 (10)
C17—H17A	0.9300	C34—H34A	0.9300
C4—O1—C3	116.0 (5)	C21—O5—C20	115.5 (5)
C7—O3—C5	118.3 (5)	C24—O7—C22	118.0 (5)
C13—O4—C10	116.9 (5)	C30—O8—C29	117.5 (5)
C2—C1—H1B	132.1	C19—C18—H18A	149.0
C1—C2—C3	174.8 (8)	C18—C19—C20	178.0 (8)
C2—C3—O1	106.5 (6)	C19—C20—O5	111.4 (6)
C2—C3—H3A	110.4	C19—C20—H20A	109.3
O1—C3—H3A	110.4	O5—C20—H20A	109.3
C2—C3—H3B	110.4	C19—C20—H20B	109.3
O1—C3—H3B	110.4	O5—C20—H20B	109.3
H3A—C3—H3B	108.6	H20A—C20—H20B	108.0
O2—C4—O1	122.0 (6)	O6—C21—O5	122.3 (6)

O2—C4—C5	126.6 (6)	O6—C21—C22	126.0 (6)
O1—C4—C5	111.4 (5)	O5—C21—C22	111.6 (6)
O3—C5—C4	109.8 (5)	O7—C22—C21	109.8 (5)
O3—C5—C6	106.1 (5)	O7—C22—C23	107.7 (5)
C4—C5—C6	111.0 (5)	C21—C22—C23	109.9 (6)
O3—C5—H5A	110.0	O7—C22—H22A	109.8
C4—C5—H5A	110.0	C21—C22—H22A	109.8
C6—C5—H5A	110.0	C23—C22—H22A	109.8
C5—C6—H6A	109.5	C22—C23—H23A	109.5
C5—C6—H6B	109.5	C22—C23—H23B	109.5
H6A—C6—H6B	109.5	H23A—C23—H23B	109.5
C5—C6—H6C	109.5	C22—C23—H23C	109.5
H6A—C6—H6C	109.5	H23A—C23—H23C	109.5
H6B—C6—H6C	109.5	H23B—C23—H23C	109.5
C12—C7—O3	115.4 (6)	C28—C24—O7	124.3 (5)
C12—C7—C8	120.7 (6)	C28—C24—C25	120.5 (5)
O3—C7—C8	123.9 (6)	O7—C24—C25	115.2 (5)
C7—C8—C9	118.5 (7)	C26—C25—C24	120.0 (6)
C7—C8—H8A	120.8	C26—C25—H25A	120.0
C9—C8—H8A	120.8	C24—C25—H25A	120.0
C10—C9—C8	120.6 (7)	C25—C26—C29	120.2 (6)
C10—C9—H9A	119.7	C25—C26—H26A	119.9
C8—C9—H9A	119.7	C29—C26—H26A	119.9
C9—C10—C11	120.8 (6)	C29—C27—C28	119.4 (6)
C9—C10—O4	118.9 (7)	C29—C27—H27A	120.3
C11—C10—O4	119.8 (7)	C28—C27—H27A	120.3
C12—C11—C10	118.8 (7)	C24—C28—C27	119.5 (6)
C12—C11—H11A	120.6	C24—C28—H28A	120.3
C10—C11—H11A	120.6	C27—C28—H28A	120.3
C7—C12—C11	120.5 (7)	C26—C29—C27	120.4 (6)
C7—C12—H12A	119.7	C26—C29—O8	121.5 (6)
C11—C12—H12A	119.7	C27—C29—O8	117.8 (6)
N1—C13—O4	121.8 (6)	N2—C30—C31	121.7 (7)
N1—C13—C14	121.8 (6)	N2—C30—O8	120.0 (5)
O4—C13—C14	116.3 (6)	C31—C30—O8	118.2 (7)
F1—C14—C15	120.8 (7)	F2—C31—C30	119.7 (7)
F1—C14—C13	119.3 (6)	F2—C31—C32	119.3 (6)
C15—C14—C13	119.8 (7)	C30—C31—C32	121.0 (8)
C16—C15—C14	117.8 (7)	C31—C32—C33	116.9 (6)
C16—C15—H15A	121.1	C31—C32—H32A	121.6
C14—C15—H15A	121.1	C33—C32—H32A	121.6
C15—C16—C17	119.1 (7)	C34—C33—C32	119.6 (7)
C15—C16—Cl1	121.6 (6)	C34—C33—Cl2	119.8 (7)
C17—C16—Cl1	119.0 (6)	C32—C33—Cl2	120.6 (6)
N1—C17—C16	122.4 (7)	C33—C34—N2	122.9 (8)
N1—C17—H17A	118.8	C33—C34—H34A	118.6
C16—C17—H17A	118.8	N2—C34—H34A	118.6
C13—N1—C17	118.7 (6)	C30—N2—C34	117.8 (6)
C4—O1—C3—C2	−168.8 (6)	C21—O5—C20—C19	−77.2 (7)

C3—O1—C4—O2	1.1 (9)	C20—O5—C21—O6	0.4 (9)
C3—O1—C4—C5	−177.8 (5)	C20—O5—C21—C22	−177.1 (6)
C7—O3—C5—C4	76.3 (7)	C24—O7—C22—C21	72.7 (7)
C7—O3—C5—C6	−163.7 (5)	C24—O7—C22—C23	−167.7 (6)
O2—C4—C5—O3	27.8 (9)	O6—C21—C22—O7	29.9 (10)
O1—C4—C5—O3	−153.4 (5)	O5—C21—C22—O7	−152.7 (5)
O2—C4—C5—C6	−89.2 (8)	O6—C21—C22—C23	−88.4 (8)
O1—C4—C5—C6	89.6 (7)	O5—C21—C22—C23	89.0 (7)
C5—O3—C7—C12	179.5 (6)	C22—O7—C24—C28	6.0 (9)
C5—O3—C7—C8	−1.3 (9)	C22—O7—C24—C25	−175.4 (6)
C12—C7—C8—C9	−2.6 (10)	C28—C24—C25—C26	1.9 (10)
O3—C7—C8—C9	178.1 (6)	O7—C24—C25—C26	−176.7 (6)
C7—C8—C9—C10	1.7 (10)	C24—C25—C26—C29	0.7 (10)
C8—C9—C10—C11	−1.0 (10)	O7—C24—C28—C27	176.3 (6)
C8—C9—C10—O4	−172.9 (5)	C25—C24—C28—C27	−2.2 (10)
C13—O4—C10—C9	−85.5 (9)	C29—C27—C28—C24	−0.1 (10)
C13—O4—C10—C11	102.5 (8)	C25—C26—C29—C27	−3.0 (10)
C9—C10—C11—C12	1.1 (9)	C25—C26—C29—O8	−176.7 (6)
O4—C10—C11—C12	172.9 (5)	C28—C27—C29—C26	2.7 (10)
O3—C7—C12—C11	−177.9 (5)	C28—C27—C29—O8	176.6 (6)
C8—C7—C12—C11	2.8 (10)	C30—O8—C29—C26	−64.8 (8)
C10—C11—C12—C7	−2.0 (9)	C30—O8—C29—C27	121.3 (7)
C10—O4—C13—N1	−2.7 (12)	C29—O8—C30—N2	−16.0 (9)
C10—O4—C13—C14	173.0 (7)	C29—O8—C30—C31	165.8 (6)
N1—C13—C14—F1	176.7 (8)	N2—C30—C31—F2	−178.3 (6)
O4—C13—C14—F1	1.0 (12)	O8—C30—C31—F2	−0.1 (10)
N1—C13—C14—C15	−2.9 (14)	N2—C30—C31—C32	3.1 (11)
O4—C13—C14—C15	−178.6 (8)	O8—C30—C31—C32	−178.7 (6)
F1—C14—C15—C16	179.5 (9)	F2—C31—C32—C33	179.9 (7)
C13—C14—C15—C16	−0.9 (15)	C30—C31—C32—C33	−1.5 (10)
C14—C15—C16—C17	4.8 (16)	C31—C32—C33—C34	−0.9 (11)
C14—C15—C16—Cl1	178.8 (8)	C31—C32—C33—Cl2	179.9 (6)
C15—C16—C17—N1	−5.4 (16)	C32—C33—C34—N2	1.8 (12)
Cl1—C16—C17—N1	−179.6 (8)	Cl2—C33—C34—N2	−179.0 (6)
O4—C13—N1—C17	178.0 (8)	C31—C30—N2—C34	−2.2 (10)
C14—C13—N1—C17	2.5 (13)	O8—C30—N2—C34	179.7 (7)
C16—C17—N1—C13	1.7 (15)	C33—C34—N2—C30	−0.2 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···F1^{i}	0.98	2.47	3.433 (9)	169
C20—H20A···N1^{ii}	0.97	2.58	3.554 (9)	179

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

Fig. 1

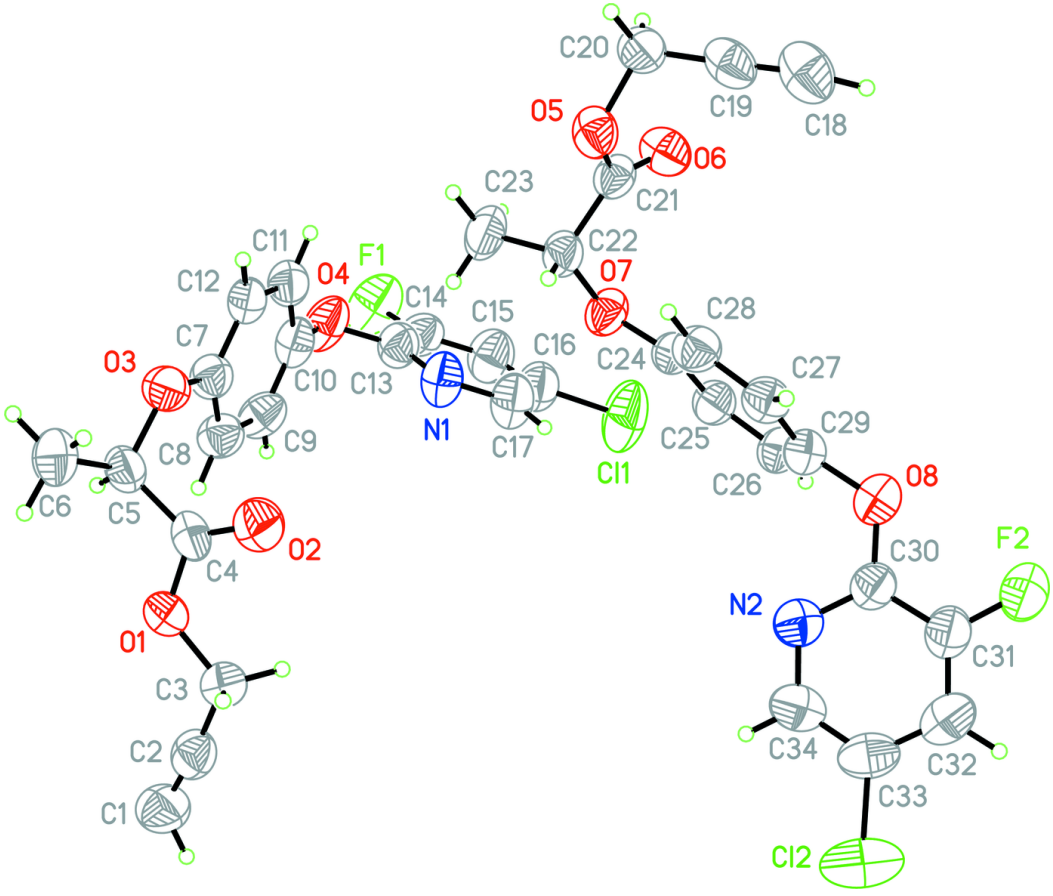
C20
C19
C18
O5
O6
C21
C23
C22
O7
C28
C24
C27
C29
O8
C26
C25
C30
F2
N2
C31
C34
C32
C33
Cl2
C11
F1
C12
O4
C14
C15
C16
C7
O3
C10
C13
N1
C17
Cl1
C9
C8
C6
C5
O2
C4
O1
C3
C2
C1

Fig. 2