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2-{4-[(*E*)-2,3-Diiodoallyl]-7-fluoro-3-oxo-3,4-dihydro-2*H*-benzo[*b*][1,4]-oxazin-6-yl}-2,3,4,5,6,7-hexahydro-1*H*-isoindole-1,3-dione

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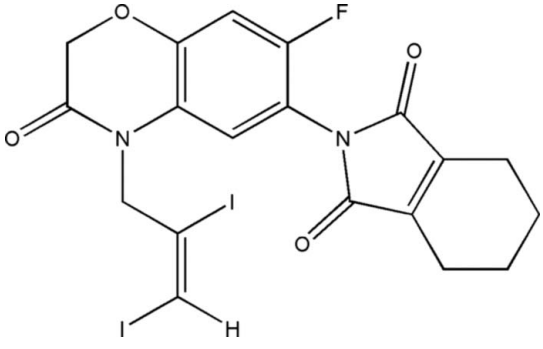
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.030; wR factor = 0.079; data-to-parameter ratio = 16.4.

In the title compound, $C_{19}H_{15}FI_2N_2O_4$, the cyclohexene and morpholinone rings adopt half-chair conformations. The dihedral angle between the benzene and pyrrole rings is 69.0 (2)°. The crystal packing is stabilized by C—H···O and C—H···F hydrogen bonds.

Related literature

For general background, see: Nair *et al.* (2003); Schallner *et al.* (2002).



Experimental

Crystal data

$C_{19}H_{15}FI_2N_2O_4$
M_r = 608.13
Monoclinic, $C2/c$
a = 23.118 (4) Å
b = 13.926 (2) Å
c = 14.975 (3) Å
β = 123.266 (2)°
V = 4030.9 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.16 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.732, T_{max} = 1.000
(expected range = 0.471–0.643)
11268 measured reflections
4138 independent reflections
3361 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.079
S = 1.01
4138 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5B···O3^{i}	0.97	2.49	3.449 (7)	171
C16—H16B···O1^{ii}	0.97	2.51	3.366 (6)	147
C17—H17B···F1^{iii}	0.97	2.53	3.256 (6)	131

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

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, 1999); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2366).

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supplementary materials

Acta Cryst. (2007). E**63**, o2742 [**doi:10.1107/S1600536807020077**]

2-{4-[(*E*)-2,3-Diiodoallyl]-7-fluoro-3-oxo-3,4-dihydro-2*H*-benzo[*b*][1,4]oxazin-6-yl}-2,3,4,5,6,7-hexahydro-1*H*-isoindole-1,3-dione

H.-L. Pang, Y. Huang, D.-L. Yin, H. Yang and W.-A. Li

Comment

Compounds containing 2*H*-benzo[b][1,4]oxazin-3(4*H*)-one groups are known to exhibit insecticidal (Nair *et al.*, 2003) and herbicidal (Schallner *et al.*, 2002) activities. As part of our investigations of the relationship between structure and bioactivity, we have synthesized a series of 2*H*-benzo[b][1,4]oxazin-3(4*H*)-one derivatives and we report here the structure of (I).

The cyclohexene ring adopts a half-chair conformation, with atoms C15 and C16 deviating from the C13/C14/C17/C18 plane by -0.192 (9) Å and 0.500 (9) Å, respectively. The morpholinone ring also adopts a half-chair conformation, with O2 and C5 deviating from the C4/C6/C11/N1 plane by -0.199 (6) and 0.344 (7) Å, respectively. The dihedral angle between the benzene and pyrrole rings is 69.0 (2)°.

The crystal packing is stabilized by intermolecular C—H···O and C—H···F hydrogen bonds (Table 1).

Experimental

Iodine (1.91 g, 7.5 mmol) was dissolved in methanol (30 ml) and the solution was added slowly to a stirred solution of 2-(7-fluoro-3-oxo-4-(prop-2-ynyl)-3,4-dihydro-2*H*-benzo[b][1,4]oxazin-6-yl)-\ 4,5,6,7-tetrahydro-2*H*-isoindole-1,3-dione (1.8 g, 5 mmol) and potassium hydroxide (0.56 g, 10 mmol) in methanol (50 ml) at room temperature. The resulting mixture was stirred for 5 h, then poured into iced water (100 ml). After filtration, the solid was washed with water and recrystallized from acetonitrile. Yellow block-shaped single crystals of (I) were obtained by evaporation of the solvent over a period of two weeks.

Refinement

H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and included in the final cycles of refinement using a riding-model, with U_{iso}(H) = 1.2U_{eq}(parent atom). The highest residual density peak is located 0.84 Å from atom I1 and the deepest hole is located 0.73 Å from atom I2.

Figures

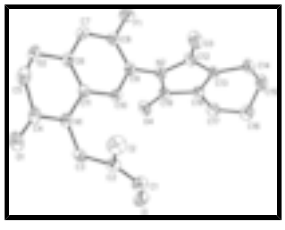


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

2-{4-[(*E*)-2,3-Diiodoallyl]-7-fluoro-3-oxo-3,4-dihydro-2*H*- benzo[*b*][1,4]oxazin-6-yl}-2,3,4,5,6,7-hexahydro-1*H*-isoindole- 1,3-dione

Crystal data

$C_{19}H_{15}FI_2N_2O_4$	F_{000} = 2320
M_r = 608.13	D_x = 2.004 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 5415 reflections
a = 23.118 (4) Å	θ = 2.7–26.3º
b = 13.926 (2) Å	μ = 3.16 mm^{-1}
c = 14.975 (3) Å	*T* = 294 (2) K
β = 123.266 (2)º	Block, yellow
V = 4030.9 (12) Å^3	0.24 × 0.20 × 0.14 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	4138 independent reflections
Radiation source: fine-focus sealed tube	3361 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −28→28
T_{min} = 0.732, T_{max} = 1.000	*k* = −17→17
11268 measured reflections	*l* = −13→18

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 9.6041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.079	$\Delta\rho_{max}$ = 1.05 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.85 e Å^{-3}
4138 reflections	Extinction correction: none
253 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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}
I1	0.085767 (14)	0.79872 (2)	0.22966 (2)	0.05341 (10)
I2	0.242669 (15)	0.56013 (2)	0.50881 (3)	0.05973 (11)
F1	0.09204 (15)	0.8397 (2)	0.7385 (2)	0.0669 (7)
O1	0.08081 (17)	0.4150 (2)	0.4174 (3)	0.0632 (8)
O2	0.06687 (15)	0.51904 (18)	0.6219 (2)	0.0504 (7)
O3	0.22865 (16)	0.9158 (2)	0.7464 (3)	0.0718 (10)
O4	0.02229 (15)	0.9427 (2)	0.4271 (2)	0.0582 (8)
N1	0.08795 (15)	0.5729 (2)	0.4618 (2)	0.0383 (7)
N2	0.11976 (15)	0.9039 (2)	0.5913 (2)	0.0383 (7)
C1	0.1654 (2)	0.7084 (3)	0.3419 (3)	0.0482 (9)
H1	0.2100	0.7189	0.3581	0.058*
C2	0.15559 (18)	0.6375 (3)	0.3907 (3)	0.0401 (8)
C3	0.08655 (19)	0.6034 (3)	0.3686 (3)	0.0404 (8)
H3A	0.0532	0.6551	0.3344	0.049*
H3B	0.0705	0.5503	0.3186	0.049*
C4	0.0862 (2)	0.4759 (3)	0.4793 (3)	0.0451 (9)
C5	0.0955 (2)	0.4511 (3)	0.5838 (4)	0.0531 (10)
H5A	0.0745	0.3890	0.5768	0.064*
H5B	0.1446	0.4449	0.6373	0.064*
C6	0.08179 (17)	0.6133 (3)	0.6143 (3)	0.0392 (8)
C7	0.0813 (2)	0.6781 (3)	0.6830 (3)	0.0469 (9)
H7	0.0733	0.6583	0.7347	0.056*
C8	0.0931 (2)	0.7739 (3)	0.6729 (3)	0.0456 (9)
C9	0.10596 (18)	0.8049 (2)	0.5982 (3)	0.0364 (7)
C10	0.10609 (17)	0.7381 (2)	0.5293 (3)	0.0351 (7)
H10	0.1151	0.7577	0.4788	0.042*
C11	0.09276 (17)	0.6418 (2)	0.5361 (3)	0.0346 (7)
C12	0.1811 (2)	0.9511 (3)	0.6655 (3)	0.0432 (9)
C13	0.17571 (19)	1.0491 (2)	0.6224 (3)	0.0391 (8)
C14	0.2311 (2)	1.1238 (3)	0.6715 (3)	0.0547 (11)
H14A	0.2717	1.1005	0.6745	0.066*
H14B	0.2442	1.1368	0.7439	0.066*
C15	0.2052 (3)	1.2164 (3)	0.6053 (4)	0.0656 (13)

H15A	0.1799	1.2538	0.6277	0.079*
H15B	0.2448	1.2542	0.6200	0.079*
C16	0.1595 (3)	1.1994 (3)	0.4877 (4)	0.0638 (12)
H16A	0.1853	1.1646	0.4643	0.077*
H16B	0.1459	1.2607	0.4509	0.077*
C17	0.0948 (2)	1.1424 (3)	0.4576 (4)	0.0539 (10)
H17A	0.0635	1.1822	0.4656	0.065*
H17B	0.0710	1.1218	0.3837	0.065*
C18	0.11612 (19)	1.0573 (2)	0.5290 (3)	0.0366 (8)
C19	0.07739 (19)	0.9643 (3)	0.5051 (3)	0.0374 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.05111 (17)	0.05720 (18)	0.05416 (17)	0.00914 (12)	0.03029 (14)	0.01610 (13)
I2	0.04430 (17)	0.0638 (2)	0.0657 (2)	0.02076 (13)	0.02673 (15)	0.01226 (14)
F1	0.100 (2)	0.0582 (15)	0.0623 (16)	−0.0063 (14)	0.0572 (16)	−0.0156 (12)
O1	0.074 (2)	0.0320 (14)	0.085 (2)	−0.0006 (14)	0.0442 (19)	−0.0107 (15)
O2	0.0565 (17)	0.0378 (14)	0.0631 (17)	−0.0050 (12)	0.0368 (15)	0.0070 (13)
O3	0.0561 (19)	0.0563 (18)	0.0576 (19)	−0.0079 (15)	0.0023 (16)	0.0142 (15)
O4	0.0465 (17)	0.0525 (17)	0.0503 (17)	−0.0066 (13)	0.0103 (14)	−0.0037 (13)
N1	0.0380 (16)	0.0302 (15)	0.0470 (17)	−0.0005 (12)	0.0235 (14)	−0.0023 (13)
N2	0.0420 (17)	0.0297 (14)	0.0382 (16)	−0.0025 (13)	0.0188 (14)	−0.0039 (12)
C1	0.039 (2)	0.058 (2)	0.051 (2)	0.0101 (18)	0.0262 (19)	0.0049 (19)
C2	0.0377 (19)	0.0395 (19)	0.041 (2)	0.0099 (15)	0.0207 (17)	−0.0019 (16)
C3	0.043 (2)	0.0351 (18)	0.0384 (19)	0.0034 (16)	0.0189 (17)	−0.0060 (15)
C4	0.039 (2)	0.0311 (18)	0.063 (2)	0.0017 (15)	0.0266 (19)	0.0030 (18)
C5	0.048 (2)	0.035 (2)	0.070 (3)	0.0056 (17)	0.029 (2)	0.0108 (19)
C6	0.0325 (18)	0.0366 (19)	0.044 (2)	−0.0026 (14)	0.0178 (16)	0.0066 (16)
C7	0.052 (2)	0.048 (2)	0.047 (2)	−0.0047 (18)	0.032 (2)	0.0025 (18)
C8	0.052 (2)	0.047 (2)	0.041 (2)	−0.0010 (18)	0.0277 (19)	−0.0043 (17)
C9	0.0359 (18)	0.0322 (17)	0.0383 (18)	−0.0012 (14)	0.0186 (16)	−0.0002 (15)
C10	0.0355 (19)	0.0335 (17)	0.0400 (19)	−0.0002 (14)	0.0230 (16)	−0.0011 (15)
C11	0.0270 (16)	0.0332 (17)	0.0387 (18)	0.0001 (13)	0.0150 (15)	−0.0006 (14)
C12	0.041 (2)	0.040 (2)	0.038 (2)	−0.0039 (16)	0.0150 (18)	−0.0032 (16)
C13	0.044 (2)	0.0317 (17)	0.0401 (19)	−0.0023 (15)	0.0224 (18)	−0.0057 (15)
C14	0.053 (2)	0.048 (2)	0.055 (2)	−0.0154 (19)	0.024 (2)	−0.0125 (19)
C15	0.074 (3)	0.044 (2)	0.080 (3)	−0.019 (2)	0.044 (3)	−0.009 (2)
C16	0.078 (3)	0.038 (2)	0.077 (3)	0.000 (2)	0.044 (3)	0.010 (2)
C17	0.057 (3)	0.045 (2)	0.054 (2)	0.0067 (19)	0.027 (2)	0.0070 (19)
C18	0.042 (2)	0.0313 (17)	0.0403 (19)	0.0014 (15)	0.0252 (17)	−0.0032 (15)
C19	0.037 (2)	0.0355 (18)	0.0386 (19)	0.0018 (15)	0.0197 (17)	−0.0067 (15)

Geometric parameters (Å, °)

I1—C1	2.098 (4)	C6—C11	1.386 (5)
I2—C2	2.106 (3)	C7—C8	1.387 (6)
F1—C8	1.352 (4)	C7—H7	0.93
O1—C4	1.211 (5)	C8—C9	1.376 (5)

O2—C6	1.377 (4)	C9—C10	1.390 (5)
O2—C5	1.440 (5)	C10—C11	1.392 (5)
O3—C12	1.207 (5)	C10—H10	0.93
O4—C19	1.202 (4)	C12—C13	1.485 (5)
N1—C4	1.381 (5)	C13—C18	1.324 (5)
N1—C11	1.426 (5)	C13—C14	1.494 (5)
N1—C3	1.443 (5)	C14—C15	1.535 (6)
N2—C19	1.395 (5)	C14—H14A	0.97
N2—C12	1.397 (5)	C14—H14B	0.97
N2—C9	1.431 (4)	C15—C16	1.494 (7)
C1—C2	1.320 (6)	C15—H15A	0.97
C1—H1	0.93	C15—H15B	0.97
C2—C3	1.518 (5)	C16—C17	1.527 (6)
C3—H3A	0.97	C16—H16A	0.97
C3—H3B	0.97	C16—H16B	0.97
C4—C5	1.498 (6)	C17—C18	1.487 (5)
C5—H5A	0.97	C17—H17A	0.97
C5—H5B	0.97	C17—H17B	0.97
C6—C7	1.374 (5)	C18—C19	1.503 (5)
C6—O2—C5	113.8 (3)	C9—C10—H10	120.0
C4—N1—C11	120.5 (3)	C11—C10—H10	120.0
C4—N1—C3	118.9 (3)	C6—C11—C10	119.2 (3)
C11—N1—C3	120.5 (3)	C6—C11—N1	119.6 (3)
C19—N2—C12	110.1 (3)	C10—C11—N1	121.1 (3)
C19—N2—C9	125.2 (3)	O3—C12—N2	125.1 (3)
C12—N2—C9	124.4 (3)	O3—C12—C13	128.6 (4)
C2—C1—I1	123.3 (3)	N2—C12—C13	106.3 (3)
C2—C1—H1	118.3	C18—C13—C12	109.2 (3)
I1—C1—H1	118.3	C18—C13—C14	125.0 (3)
C1—C2—C3	126.4 (3)	C12—C13—C14	125.5 (3)
C1—C2—I2	118.2 (3)	C13—C14—C15	110.0 (4)
C3—C2—I2	115.4 (3)	C13—C14—H14A	109.7
N1—C3—C2	114.7 (3)	C15—C14—H14A	109.7
N1—C3—H3A	108.6	C13—C14—H14B	109.7
C2—C3—H3A	108.6	C15—C14—H14B	109.7
N1—C3—H3B	108.6	H14A—C14—H14B	108.2
C2—C3—H3B	108.6	C16—C15—C14	113.6 (4)
H3A—C3—H3B	107.6	C16—C15—H15A	108.8
O1—C4—N1	122.8 (4)	C14—C15—H15A	108.8
O1—C4—C5	122.3 (4)	C16—C15—H15B	108.8
N1—C4—C5	114.9 (3)	C14—C15—H15B	108.8
O2—C5—C4	115.4 (3)	H15A—C15—H15B	107.7
O2—C5—H5A	108.4	C15—C16—C17	112.1 (4)
C4—C5—H5A	108.4	C15—C16—H16A	109.2
O2—C5—H5B	108.4	C17—C16—H16A	109.2
C4—C5—H5B	108.4	C15—C16—H16B	109.2
H5A—C5—H5B	107.5	C17—C16—H16B	109.2
C7—C6—O2	117.3 (3)	H16A—C16—H16B	107.9
C7—C6—C11	121.7 (3)	C18—C17—C16	108.5 (3)

O2—C6—C11	120.9 (3)	C18—C17—H17A	110.0
C6—C7—C8	117.9 (4)	C16—C17—H17A	110.0
C6—C7—H7	121.1	C18—C17—H17B	110.0
C8—C7—H7	121.1	C16—C17—H17B	110.0
F1—C8—C9	118.4 (4)	H17A—C17—H17B	108.4
F1—C8—C7	119.3 (3)	C13—C18—C17	124.8 (3)
C9—C8—C7	122.3 (4)	C13—C18—C19	108.4 (3)
C8—C9—C10	118.9 (3)	C17—C18—C19	126.6 (3)
C8—C9—N2	121.2 (3)	O4—C19—N2	125.5 (3)
C10—C9—N2	120.0 (3)	O4—C19—C18	128.5 (4)
C9—C10—C11	120.0 (3)	N2—C19—C18	106.0 (3)
I1—C1—C2—C3	5.7 (6)	C9—C10—C11—C6	−2.2 (5)
I1—C1—C2—I2	−175.86 (18)	C9—C10—C11—N1	175.7 (3)
C4—N1—C3—C2	−104.5 (4)	C4—N1—C11—C6	−12.9 (5)
C11—N1—C3—C2	74.0 (4)	C3—N1—C11—C6	168.6 (3)
C1—C2—C3—N1	−143.5 (4)	C4—N1—C11—C10	169.2 (3)
I2—C2—C3—N1	38.0 (4)	C3—N1—C11—C10	−9.3 (5)
C11—N1—C4—O1	178.6 (3)	C19—N2—C12—O3	−177.3 (4)
C3—N1—C4—O1	−3.0 (6)	C9—N2—C12—O3	−3.1 (6)
C11—N1—C4—C5	−4.8 (5)	C19—N2—C12—C13	0.9 (4)
C3—N1—C4—C5	173.7 (3)	C9—N2—C12—C13	175.1 (3)
C6—O2—C5—C4	−45.6 (5)	O3—C12—C13—C18	177.0 (4)
O1—C4—C5—O2	−149.4 (4)	N2—C12—C13—C18	−1.1 (4)
N1—C4—C5—O2	33.9 (5)	O3—C12—C13—C14	2.0 (7)
C5—O2—C6—C7	−155.2 (4)	N2—C12—C13—C14	−176.1 (4)
C5—O2—C6—C11	28.5 (5)	C18—C13—C14—C15	7.4 (6)
O2—C6—C7—C8	−177.1 (3)	C12—C13—C14—C15	−178.3 (4)
C11—C6—C7—C8	−0.8 (6)	C13—C14—C15—C16	−36.9 (6)
C6—C7—C8—F1	179.2 (3)	C14—C15—C16—C17	60.0 (6)
C6—C7—C8—C9	−1.0 (6)	C15—C16—C17—C18	−48.6 (5)
F1—C8—C9—C10	−179.1 (3)	C12—C13—C18—C17	−174.8 (4)
C7—C8—C9—C10	1.1 (6)	C14—C13—C18—C17	0.3 (6)
F1—C8—C9—N2	1.6 (6)	C12—C13—C18—C19	0.8 (4)
C7—C8—C9—N2	−178.3 (4)	C14—C13—C18—C19	175.9 (4)
C19—N2—C9—C8	−114.3 (4)	C16—C17—C18—C13	20.0 (6)
C12—N2—C9—C8	72.4 (5)	C16—C17—C18—C19	−154.8 (4)
C19—N2—C9—C10	66.3 (5)	C12—N2—C19—O4	177.5 (4)
C12—N2—C9—C10	−107.0 (4)	C9—N2—C19—O4	3.3 (6)
C8—C9—C10—C11	0.5 (5)	C12—N2—C19—C18	−0.4 (4)
N2—C9—C10—C11	179.9 (3)	C9—N2—C19—C18	−174.6 (3)
C7—C6—C11—C10	2.3 (5)	C13—C18—C19—O4	−178.1 (4)
O2—C6—C11—C10	178.5 (3)	C17—C18—C19—O4	−2.6 (6)
C7—C6—C11—N1	−175.6 (3)	C13—C18—C19—N2	−0.3 (4)
O2—C6—C11—N1	0.6 (5)	C17—C18—C19—N2	175.2 (4)

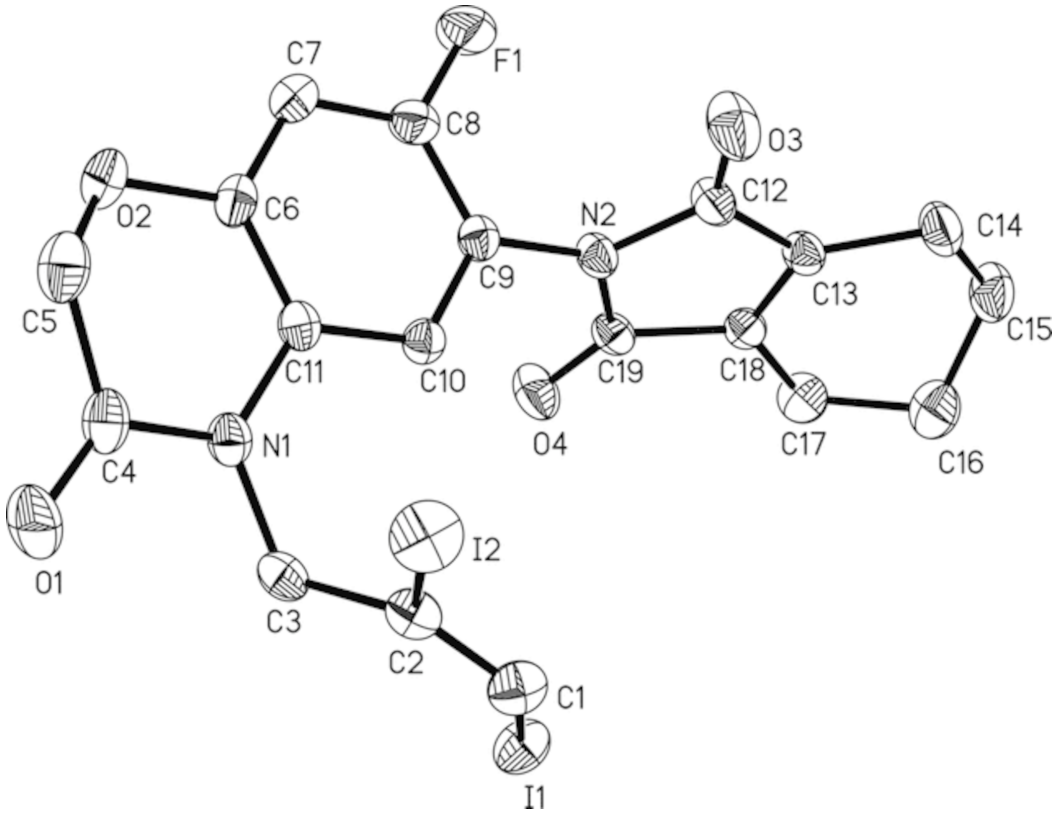
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5B···O3^{i}	0.97	2.49	3.449 (7)	171

C16—H16B···O1^{ii}	0.97	2.51	3.366 (6)	147
C17—H17B···F1^{iii}	0.97	2.53	3.256 (6)	131

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

Fig. 1


C7
F1
C8
O3
C12
O2
C6
N2
C14
C9
C13
C5
C15
C11
C10
C19
C18
O4
C17
C16
N1
C4
I2
O1
C3
C2
C1
I1