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Crystal structure of flumioxazin

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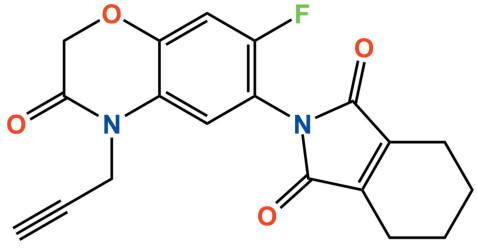
The title compound {systematic name: 2-[7-fluoro-3,4-dihydro-3-oxo-4-(prop-2-yn-1-yl)-2*H*-1,4-benzoxazin-6-yl]-4,5,6,7-tetrahydro-1*H*-isoindole-1,3(2*H*)-dione}, $C_{19}H_{15}FN_2O_4$, is a dicarboximide herbicide. The dihedral angle between the maleimide and benzene ring planes is 66.13 (5)°. In the crystal, C—H···O and C—H···F hydrogen bonds and weak C—H···π interactions [3.5601 (19) Å] link adjacent molecules, forming two-dimensional networks extending parallel to the (110) plane.

Keywords: crystal structure; dicarboximide herbicide; flumioxazin; 1*H*-isoindole; 1,4-benzoxazine; C—H···F hydrogen bonds.

CCDC reference: 1424397

1. Related literature

For information on the herbicidal properties of the title compound, see: Saladin *et al.* (2003); Geoffroy *et al.* (2004). For a related crystal structure, see: Hou *et al.* (2004).



2. Experimental

2.1. Crystal data

$C_{19}H_{15}FN_2O_4$
M_r = 354.33
Monoclinic, $P2_1/c$
a = 8.896 (1) Å
b = 7.1592 (8) Å
c = 25.708 (3) Å
β = 96.039 (6)°
V = 1628.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 173 K
0.50 × 0.26 × 0.05 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.575, T_{max} = 0.746
27372 measured reflections
4067 independent reflections
3277 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.137
S = 1.07
4067 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

*Cg*1 is the centroid of the C3/C4/C8–C11 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O4^{i}	0.95	2.39	3.178 (2)	140
C19—H19*B*···F1^{ii}	0.99	2.36	3.289 (2)	155
C16—H16*A*···*Cg*1^{iii}	0.99	2.63	3.5601 (19)	157

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

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7502).

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supporting information

Acta Cryst. (2015). E**71**, o768 [doi:10.1107/S2056989015017223]

Crystal structure of flumioxazin

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S1. Comment

Flumioxazin [systematic name: 2-[7-fluoro-3,4-dihydro-3-oxo-4-(2-propyn-1-yl)-2*H*-1,4-benzoxazin-6-yl]-4,5,6,7-tetrahydro-1*H*-isoindole-1,3(2*H*)-dione] is a soil applied pre-emergent herbicide used to inhibit development of redroot pigweed. (Geoffroy *et al.*, 2004; Saladin *et al.*, 2003). However, its crystal structure has not been reported until now. In the title compound (Fig. 1), the dihedral angle between pyrrole and benzne rings is 66.13 (5)°. All bond lengths and bond angles are normal and comparable to those observed in a similar crystal structure (Hou *et al.*, 2004).

In the crystal structure (Fig. 2), C—H···O and C—H···F hydrogen bonds and weak C–H···π interactions are observed (Table 1). Two-dimensional networks are formed by the hydrogen bonds and weak C–H···π interactions.

S2. Experimental

The title compound was purchased from the Dr Ehrenstorfer GmbH Company. Slow evaporation of a solution in CH_3CN gave single crystals suitable for X-ray analysis.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.99 Å, U_{iso} = 1.2U_{eq}(C) for CH_2 group, d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for aromatic C—H aromatic C—H and C*sp*—H.

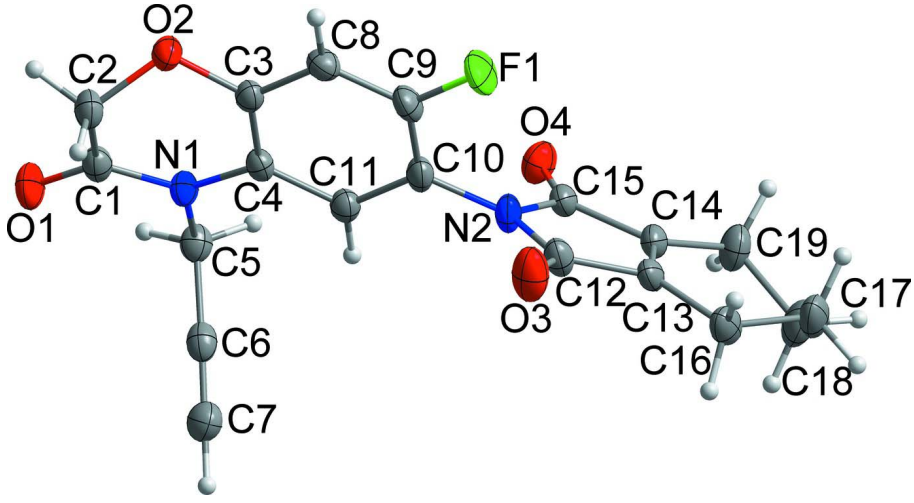

Figure 1

The asymmetric unit of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

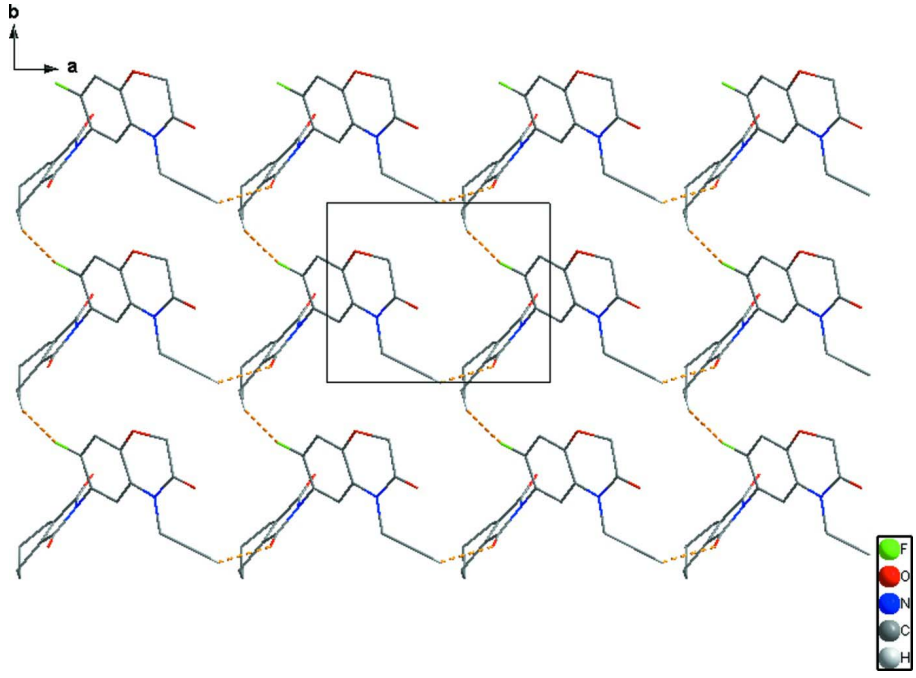

Figure 2

Crystal packing viewed along the *c* axis. The intermolecular interactions are shown as dashed lines.

2-[7-Fluoro-3,4-dihydro-3-oxo-4-(prop-2-yn-1-yl)-2*H*-1,4-benzoxazin-6-yl]-4,5,6,7-tetrahydro-1*H*-isoindole-1,3(2*H*)-dione

Crystal data

$C_{19}H_{15}FN_2O_4$
$M_r = 354.33$
Monoclinic, $P2_1/c$
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$b = 7.1592$ (8) Å
$c = 25.708$ (3) Å
$\beta = 96.039$ (6)°
$V = 1628.2$ (3) Å^3
$Z = 4$
$F(000) = 736$
$D_x = 1.445$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8497 reflections
$\theta = 2.7$–$28.2°$
$\mu = 0.11$ mm^{-1}
$T = 173$ K
Plate, colourless
0.50 × 0.26 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min} = 0.575$, $T_{max} = 0.746$
27372 measured reflections
4067 independent reflections
3277 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.6°$
$h = -11 \rightarrow 11$
$k = -9 \rightarrow 9$
$l = -34 \rightarrow 34$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.137$
$S = 1.07$
4067 reflections
235 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.9028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.77768 (12)	0.66568 (18)	0.33755 (5)	0.0431 (3)
O1	1.40190 (15)	0.41585 (19)	0.54636 (5)	0.0359 (3)
O2	1.12467 (13)	0.73087 (17)	0.48786 (4)	0.0273 (3)
O3	0.94166 (16)	0.4892 (2)	0.25135 (5)	0.0459 (4)
O4	0.74322 (15)	0.08897 (18)	0.36415 (5)	0.0331 (3)
N1	1.22083 (15)	0.3652 (2)	0.47885 (5)	0.0235 (3)
N2	0.86942 (16)	0.3094 (2)	0.31951 (5)	0.0276 (3)
C1	1.30559 (18)	0.4767 (3)	0.51371 (6)	0.0265 (4)
C2	1.27631 (19)	0.6824 (3)	0.50845 (7)	0.0291 (4)
H2A	1.2983	0.7410	0.5433	0.035*
H2B	1.3474	0.7360	0.4853	0.035*
C3	1.06753 (17)	0.6259 (2)	0.44577 (6)	0.0226 (3)
C4	1.11458 (17)	0.4423 (2)	0.43988 (6)	0.0217 (3)
C5	1.2461 (2)	0.1636 (2)	0.48166 (6)	0.0272 (4)
H5A	1.1481	0.0987	0.4739	0.033*
H5B	1.2872	0.1300	0.5177	0.033*
C6	1.3508 (2)	0.0983 (2)	0.44508 (7)	0.0284 (4)
C7	1.4371 (2)	0.0447 (3)	0.41648 (7)	0.0357 (4)
H7	1.5064	0.0015	0.3935	0.043*
C8	0.95463 (18)	0.7036 (3)	0.41121 (6)	0.0266 (4)
H8	0.9225	0.8288	0.4154	0.032*
C9	0.89012 (18)	0.5945 (3)	0.37066 (7)	0.0284 (4)
C10	0.93760 (18)	0.4142 (3)	0.36273 (6)	0.0261 (4)
C11	1.05195 (18)	0.3384 (2)	0.39736 (6)	0.0244 (3)
H11	1.0873	0.2154	0.3920	0.029*
C12	0.87139 (19)	0.3604 (3)	0.26659 (7)	0.0298 (4)
C13	0.76914 (17)	0.2264 (3)	0.23609 (6)	0.0252 (4)
C14	0.70932 (18)	0.1121 (2)	0.26880 (6)	0.0246 (4)
C15	0.77039 (17)	0.1593 (2)	0.32346 (6)	0.0235 (3)
C16	0.7429 (2)	0.2189 (3)	0.17802 (6)	0.0338 (4)
H16A	0.8355	0.1746	0.1637	0.041*
H16B	0.7193	0.3457	0.1640	0.041*
C17	0.6125 (2)	0.0878 (3)	0.16111 (7)	0.0430 (5)
H17A	0.5158	0.1542	0.1634	0.052*

H17B	0.6171	0.0519	0.1241	0.052*
C18	0.6158 (3)	−0.0865 (3)	0.19432 (8)	0.0468 (5)
H18A	0.7113	−0.1546	0.1912	0.056*
H18B	0.5311	−0.1690	0.1809	0.056*
C19	0.6033 (2)	−0.0436 (3)	0.25236 (7)	0.0361 (4)
H19A	0.4984	−0.0070	0.2573	0.043*
H19B	0.6297	−0.1559	0.2739	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0319 (6)	0.0490 (7)	0.0443 (6)	0.0126 (5)	−0.0160 (5)	−0.0011 (5)
O1	0.0353 (7)	0.0380 (8)	0.0310 (6)	−0.0010 (6)	−0.0128 (5)	0.0025 (6)
O2	0.0270 (6)	0.0264 (6)	0.0273 (6)	−0.0010 (5)	−0.0021 (5)	−0.0052 (5)
O3	0.0433 (8)	0.0572 (10)	0.0362 (7)	−0.0243 (7)	−0.0003 (6)	0.0082 (7)
O4	0.0408 (7)	0.0352 (7)	0.0228 (6)	−0.0063 (6)	0.0011 (5)	0.0015 (5)
N1	0.0241 (7)	0.0220 (7)	0.0230 (6)	0.0000 (6)	−0.0034 (5)	0.0015 (5)
N2	0.0235 (7)	0.0368 (8)	0.0213 (6)	−0.0068 (6)	−0.0036 (5)	−0.0004 (6)
C1	0.0234 (8)	0.0334 (9)	0.0222 (7)	−0.0031 (7)	−0.0004 (6)	0.0009 (7)
C2	0.0264 (8)	0.0290 (9)	0.0301 (8)	−0.0042 (7)	−0.0055 (7)	−0.0026 (7)
C3	0.0197 (7)	0.0258 (8)	0.0222 (7)	−0.0031 (6)	0.0012 (6)	−0.0014 (6)
C4	0.0174 (7)	0.0247 (8)	0.0224 (7)	−0.0019 (6)	0.0001 (6)	0.0022 (6)
C5	0.0296 (8)	0.0247 (9)	0.0263 (8)	−0.0005 (7)	−0.0016 (6)	0.0027 (7)
C6	0.0288 (8)	0.0234 (9)	0.0309 (8)	−0.0005 (7)	−0.0065 (7)	0.0005 (7)
C7	0.0341 (10)	0.0369 (11)	0.0354 (9)	−0.0024 (8)	0.0004 (8)	−0.0058 (8)
C8	0.0221 (8)	0.0269 (9)	0.0306 (8)	0.0032 (7)	0.0020 (6)	0.0001 (7)
C9	0.0196 (8)	0.0354 (10)	0.0289 (8)	0.0028 (7)	−0.0041 (6)	0.0036 (7)
C10	0.0208 (8)	0.0332 (9)	0.0235 (7)	−0.0050 (7)	−0.0018 (6)	−0.0023 (7)
C11	0.0220 (8)	0.0263 (8)	0.0245 (7)	−0.0026 (7)	0.0007 (6)	−0.0008 (7)
C12	0.0221 (8)	0.0410 (10)	0.0255 (8)	−0.0046 (8)	−0.0010 (6)	0.0024 (7)
C13	0.0176 (7)	0.0355 (9)	0.0217 (7)	0.0024 (7)	−0.0022 (6)	−0.0006 (7)
C14	0.0204 (7)	0.0300 (9)	0.0221 (7)	0.0014 (7)	−0.0031 (6)	−0.0020 (6)
C15	0.0192 (7)	0.0280 (8)	0.0226 (7)	0.0017 (6)	−0.0013 (6)	−0.0010 (6)
C16	0.0285 (9)	0.0515 (12)	0.0207 (8)	0.0011 (8)	−0.0011 (6)	0.0025 (8)
C17	0.0322 (10)	0.0718 (15)	0.0234 (8)	−0.0059 (10)	−0.0039 (7)	−0.0085 (9)
C18	0.0483 (12)	0.0536 (14)	0.0368 (10)	−0.0122 (10)	−0.0032 (9)	−0.0155 (10)
C19	0.0397 (10)	0.0367 (11)	0.0301 (9)	−0.0123 (9)	−0.0047 (7)	−0.0025 (8)

Geometric parameters (Å, º)

F1—C9	1.3436 (19)	C7—H7	0.9500
O1—C1	1.215 (2)	C8—C9	1.378 (2)
O2—C3	1.3707 (19)	C8—H8	0.9500
O2—C2	1.439 (2)	C9—C10	1.380 (3)
O3—C12	1.203 (2)	C10—C11	1.390 (2)
O4—C15	1.208 (2)	C11—H11	0.9500
N1—C1	1.366 (2)	C12—C13	1.487 (2)
N1—C4	1.4153 (19)	C13—C14	1.325 (2)

N1—C5	1.461 (2)	C13—C16	1.488 (2)
N2—C15	1.400 (2)	C14—C15	1.491 (2)
N2—C12	1.410 (2)	C14—C19	1.493 (2)
N2—C10	1.422 (2)	C16—C17	1.520 (3)
C1—C2	1.499 (3)	C16—H16A	0.9900
C2—H2A	0.9900	C16—H16B	0.9900
C2—H2B	0.9900	C17—C18	1.511 (3)
C3—C8	1.386 (2)	C17—H17A	0.9900
C3—C4	1.392 (2)	C17—H17B	0.9900
C4—C11	1.390 (2)	C18—C19	1.539 (3)
C5—C6	1.468 (2)	C18—H18A	0.9900
C5—H5A	0.9900	C18—H18B	0.9900
C5—H5B	0.9900	C19—H19A	0.9900
C6—C7	1.182 (3)	C19—H19B	0.9900

C3—O2—C2	114.43 (13)	C4—C11—C10	120.04 (16)
C1—N1—C4	121.20 (14)	C4—C11—H11	120.0
C1—N1—C5	118.24 (14)	C10—C11—H11	120.0
C4—N1—C5	120.54 (13)	O3—C12—N2	124.88 (16)
C15—N2—C12	109.88 (13)	O3—C12—C13	129.26 (16)
C15—N2—C10	124.61 (14)	N2—C12—C13	105.84 (14)
C12—N2—C10	124.73 (15)	C14—C13—C12	109.15 (14)
O1—C1—N1	122.97 (17)	C14—C13—C16	125.71 (16)
O1—C1—C2	121.16 (16)	C12—C13—C16	125.12 (16)
N1—C1—C2	115.85 (14)	C13—C14—C15	109.11 (15)
O2—C2—C1	114.67 (14)	C13—C14—C19	124.47 (15)
O2—C2—H2A	108.6	C15—C14—C19	126.37 (15)
C1—C2—H2A	108.6	O4—C15—N2	124.57 (15)
O2—C2—H2B	108.6	O4—C15—C14	129.44 (16)
C1—C2—H2B	108.6	N2—C15—C14	105.98 (13)
H2A—C2—H2B	107.6	C13—C16—C17	110.12 (15)
O2—C3—C8	117.99 (15)	C13—C16—H16A	109.6
O2—C3—C4	120.85 (14)	C17—C16—H16A	109.6
C8—C3—C4	121.02 (15)	C13—C16—H16B	109.6
C11—C4—C3	119.39 (14)	C17—C16—H16B	109.6
C11—C4—N1	122.06 (15)	H16A—C16—H16B	108.2
C3—C4—N1	118.50 (14)	C18—C17—C16	112.33 (16)
N1—C5—C6	112.80 (14)	C18—C17—H17A	109.1
N1—C5—H5A	109.0	C16—C17—H17A	109.1
C6—C5—H5A	109.0	C18—C17—H17B	109.1
N1—C5—H5B	109.0	C16—C17—H17B	109.1
C6—C5—H5B	109.0	H17A—C17—H17B	107.9
H5A—C5—H5B	107.8	C17—C18—C19	112.57 (18)
C7—C6—C5	178.63 (19)	C17—C18—H18A	109.1
C6—C7—H7	180.0	C19—C18—H18A	109.1
C9—C8—C3	118.25 (16)	C17—C18—H18B	109.1
C9—C8—H8	120.9	C19—C18—H18B	109.1
C3—C8—H8	120.9	H18A—C18—H18B	107.8

F1—C9—C8	119.17 (16)	C14—C19—C18	108.39 (16)
F1—C9—C10	118.68 (15)	C14—C19—H19A	110.0
C8—C9—C10	122.15 (15)	C18—C19—H19A	110.0
C9—C10—C11	119.04 (15)	C14—C19—H19B	110.0
C9—C10—N2	119.79 (15)	C18—C19—H19B	110.0
C11—C10—N2	121.17 (16)	H19A—C19—H19B	108.4
C4—N1—C1—O1	−177.07 (15)	C3—C4—C11—C10	−3.5 (2)
C5—N1—C1—O1	0.9 (2)	N1—C4—C11—C10	173.89 (14)
C4—N1—C1—C2	1.1 (2)	C9—C10—C11—C4	1.4 (2)
C5—N1—C1—C2	179.13 (15)	N2—C10—C11—C4	−178.70 (15)
C3—O2—C2—C1	−44.1 (2)	C15—N2—C12—O3	177.05 (18)
O1—C1—C2—O2	−152.56 (16)	C10—N2—C12—O3	6.8 (3)
N1—C1—C2—O2	29.2 (2)	C15—N2—C12—C13	−1.89 (19)
C2—O2—C3—C8	−154.71 (15)	C10—N2—C12—C13	−172.15 (15)
C2—O2—C3—C4	29.4 (2)	O3—C12—C13—C14	−176.9 (2)
O2—C3—C4—C11	178.59 (14)	N2—C12—C13—C14	1.96 (19)
C8—C3—C4—C11	2.9 (2)	O3—C12—C13—C16	5.0 (3)
O2—C3—C4—N1	1.1 (2)	N2—C12—C13—C16	−176.16 (16)
C8—C3—C4—N1	−174.58 (14)	C12—C13—C14—C15	−1.26 (19)
C1—N1—C4—C11	165.50 (15)	C16—C13—C14—C15	176.84 (16)
C5—N1—C4—C11	−12.5 (2)	C12—C13—C14—C19	−178.74 (16)
C1—N1—C4—C3	−17.1 (2)	C16—C13—C14—C19	−0.6 (3)
C5—N1—C4—C3	164.92 (15)	C12—N2—C15—O4	−178.20 (17)
C1—N1—C5—C6	−95.61 (17)	C10—N2—C15—O4	−7.9 (3)
C4—N1—C5—C6	82.40 (19)	C12—N2—C15—C14	1.17 (18)
O2—C3—C8—C9	−176.00 (15)	C10—N2—C15—C14	171.45 (15)
C4—C3—C8—C9	−0.2 (2)	C13—C14—C15—O4	179.43 (18)
C3—C8—C9—F1	178.24 (15)	C19—C14—C15—O4	−3.2 (3)
C3—C8—C9—C10	−2.0 (3)	C13—C14—C15—N2	0.10 (19)
F1—C9—C10—C11	−178.83 (15)	C19—C14—C15—N2	177.52 (16)
C8—C9—C10—C11	1.4 (3)	C14—C13—C16—C17	11.8 (3)
F1—C9—C10—N2	1.2 (2)	C12—C13—C16—C17	−170.41 (17)
C8—C9—C10—N2	−178.51 (16)	C13—C16—C17—C18	−40.6 (2)
C15—N2—C10—C9	−108.0 (2)	C16—C17—C18—C19	60.9 (2)
C12—N2—C10—C9	60.9 (2)	C13—C14—C19—C18	17.6 (3)
C15—N2—C10—C11	72.1 (2)	C15—C14—C19—C18	−159.46 (17)
C12—N2—C10—C11	−119.05 (19)	C17—C18—C19—C14	−46.4 (2)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C3/C4/C8–C11 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O4^{i}	0.95	2.39	3.178 (2)	140
C19—H19*B*···F1^{ii}	0.99	2.36	3.289 (2)	155
C16—H16*A*···*Cg*1^{iii}	0.99	2.63	3.5601 (19)	157

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