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1,1-Difluoro-3-phenyl-9-(pyridin-2-yl)-1*H*-1λ^4,11λ^4-1,3,5,2-oxadiazaborinino[3,4-*a*][1,8]-naphthyridine

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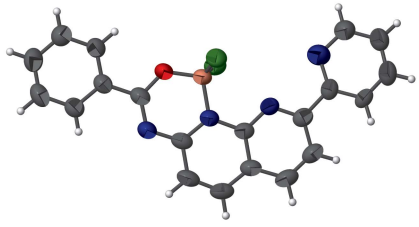
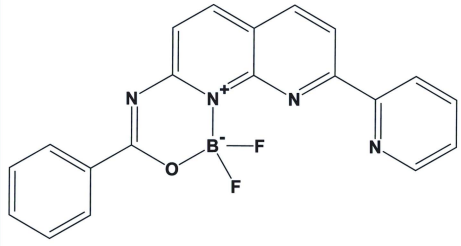
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{13}BF_2N_4O$, the central fused three-ring oxadiazaborininonaphthyridine system is planar (r.m.s. deviation of 0.03 Å). The phenyl ring lies in the plane of this ring system, making a dihedral angle of 0.61 (14)°, and is inclined to the pyridine ring by 9.02 (19)°. In the crystal, molecules are connected by C—H···F hydrogen bonds, forming chains propagating along the *b*-axis direction. The chains are linked by offset π–π interactions [intercentroid distance = 3.4550 (13) Å], forming a three-dimensional supramolecular architecture.

3D view



Chemical scheme



Structure description

Over the past decade, BF_2 complexes have been known to be fluorescent dyes with high fluorescence quantum yields (Zheng *et al.*, 2015), sharp fluorescence peaks (Du *et al.*, 2014), high extinction coefficients (Kubota *et al.*, 2010) and high chemical stability (Li *et al.*, 2010). They are widely applied as sensors (Gonçalves, 2009; Kobayashi *et al.*, 2010; Tachikawa *et al.*, 2010), photodynamic therapy agents (Lovell *et al.*, 2010; Ozlem & Akkaya, 2009), photo-electric materials (Gomez-Duran *et al.*, 2010; Lovell *et al.*, 2010; Ortiz *et al.*, 2010; Ozlem & Akkaya, 2008) and light-harvesting materials (Erten-Ela *et al.*, 2008; Rousseau *et al.*, 2009). 1,8-Naphthyridines have attracted interest due to their diverse coordination modes and have been used as ion probes (Liu *et al.*, 2014), as luminescent materials (Li *et al.*, 2014) and in biochemistry (Zhao *et al.*, 2014). The above observations prompted us to synthesize the title compound, which is a novel BF_2 complex based on a 1,8-naphthyridine derivative, and we report herein on its crystal structure.

The molecular structure of the title compound is shown in Fig. 1. It contains naphthyridine, pyridyl and phenyl rings. The naphthyridine ring system is fused with a di-

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···F2^{i}	0.93	2.47	3.353 (4)	160

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

fluororoxadiazaborinino unit. The fused oxadiazaborininonaphthyridine ring system is planar (r.m.s. deviation of 0.03 Å). The phenyl ring (C1–C6) lies in the plane of this ring system, making a dihedral angle of 0.61 (14)°, and is inclined to the pyridine ring (N4/C16–C20) by 9.02 (19)°.

In the crystal, molecules are linked by C—H···F hydrogen bonds, forming chains along the *b*-axis direction (Fig. 2 and Table 1). The chains are linked *via* offset π–π interactions [$Cg2\cdots Cg5^{i}$ = 3.519 (2) Å, interplanar distance = 3.4550 (13) Å, slippage = 0.629 Å; $Cg2$ and $Cg5$ are the centroids of rings N2/C8–C11/C15 and C1–C6, respectively; symmetry code: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$], forming a three-dimensional supramolecular architecture (Fig. 3).

Owing to the shortage of BF_2 complexes based on 1,8-naphthyridine derivatives, there are few examples of similar compounds in the literature. A search of the Cambridge

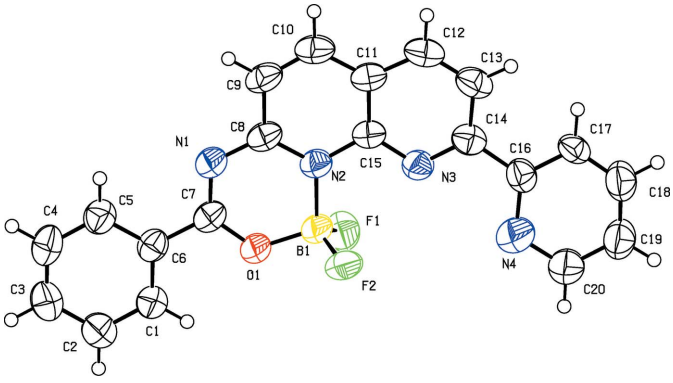


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level

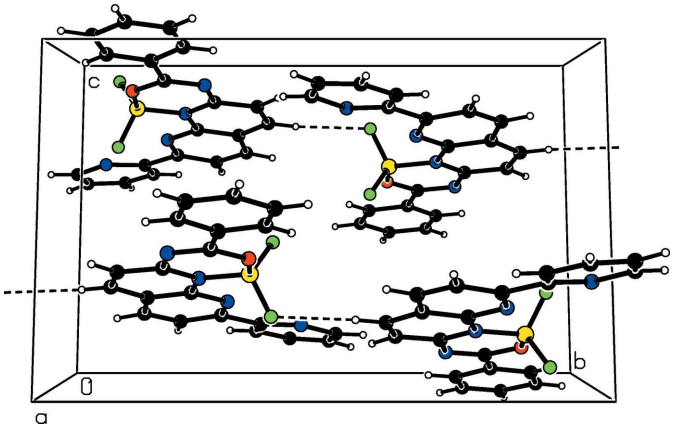


Figure 2
A view along the *a* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (Table 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{13}BF_2N_4O$
M_r	374.15
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	10.144 (2), 16.276 (3), 10.491 (2)
β (°)	101.27 (3)
V (Å^3)	1698.8 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.28 × 0.26 × 0.24
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.970, 0.975
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14275, 3328, 1795
R_{int}	0.058
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.233, 1.05
No. of reflections	3328
No. of parameters	253
No. of restraints	4
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.36

Computer programs: *PROCESS-AUTO* (Rigaku, 1998), *CrystalStructure* (Rigaku/MSC, 2006), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

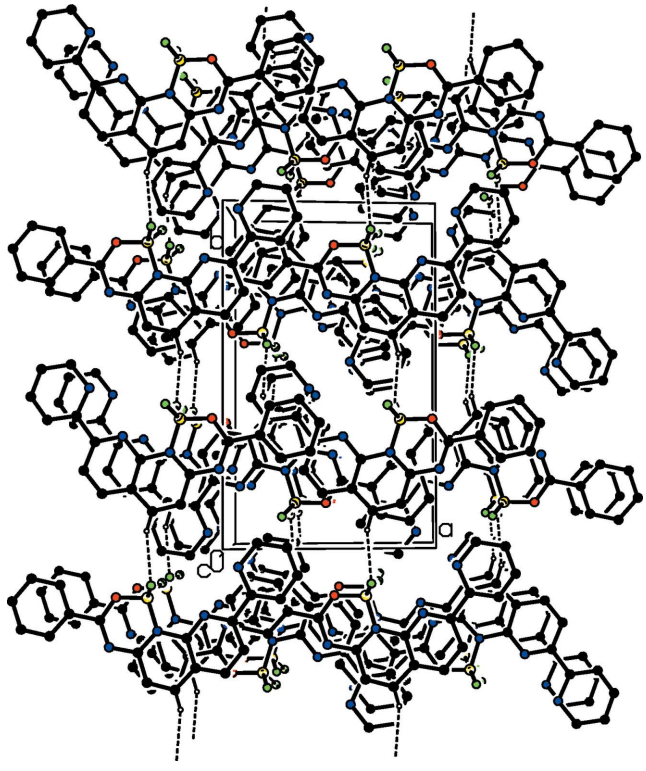


Figure 3
A view along the *c* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (Table 1) and, of the H atoms, only H10 is shown for clarity.

Structural Database (Version 5.37, November 2015; Groom *et al.*, 2016) revealed the structure of one very similar compound *viz*. 1,1-difluoro-7,9-dimethyl-3-phenyl-1*H*-[1,3,5,2]oxadiazaborinino-[3,4-*a*][1,8] naphthyridin-11-ium-1-uide (Wu *et al.*, 2012).

Synthesis and crystallization

$BF_3{\cdot}OEt_2$ (2 ml, 16 mmol) was added dropwise to an ice-cooled solution of 2,6-lutidine (1 ml) and *N*-[7-(pyridin-2-yl)-1,8-naphthyridin-2-yl]benzamide (0.326 g,1 mmol) in anhydrous CH_2Cl_2 (80 ml) under a nitrogen atmosphere. After the mixture was stirred for 24 h at room temperature, the reaction was quenched by 20 ml distilled water. The aqueous layer was extracted with CH_2Cl_2 (3 × 100 ml), the organic layer was dried with Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by silica gel chromatography using CH_2Cl_2 as eluent to give the pure product as a bright-yellow powder (yield 0.184 g, 50%). Crystals of the title compound were obtained from the CH_2Cl_2 solution by slow evaporation of the solvent at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161129 [https://doi.org/10.1107/S2414314616011299]

1,1-Difluoro-3-phenyl-9-(pyridin-2-yl)-1*H*-1λ^4,11λ^4-1,3,5,2-oxadiazaborinino[3,4-*a*][1,8]naphthyridine

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1,1-Difluoro-3-phenyl-9-(pyridin-2-yl)-1*H*-1λ^4,11λ^4-1,3,5,2-oxadiazaborinino[3,4-*a*][1,8]naphthyridine

Crystal data

$C_{20}H_{13}BF_2N_4O$
M_r = 374.15
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.144 (2) Å
b = 16.276 (3) Å
c = 10.491 (2) Å
β = 101.27 (3)°
V = 1698.8 (6) Å^3
Z = 4
$F(000)$ = 768
D_x = 1.463 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3328 reflections
θ = 3.1–26.0°
μ = 0.11 mm^{-1}
T = 293 K
Blcok, yellow
0.28 × 0.26 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.970, T_{max} = 0.975
14275 measured reflections
3328 independent reflections
1795 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 26.0°, θ_{min} = 3.1°
h = −12→12
k = −20→20
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.233
S = 1.05
3328 reflections
253 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1317P)^2 + 0.0306P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
B1	0.3307 (4)	0.1319 (2)	0.8391 (4)	0.0577 (10)
F1	0.27253 (19)	0.09215 (12)	0.9281 (2)	0.0773 (7)
F2	0.3042 (2)	0.09408 (11)	0.7184 (2)	0.0786 (7)
N1	0.5098 (3)	0.27104 (16)	0.9010 (3)	0.0570 (7)
N2	0.2844 (3)	0.22483 (15)	0.8257 (2)	0.0504 (7)
N3	0.0659 (3)	0.17947 (15)	0.7507 (3)	0.0535 (7)
N4	−0.0920 (3)	0.0434 (2)	0.6740 (4)	0.0949 (12)
O1	0.4774 (2)	0.13081 (12)	0.8848 (3)	0.0672 (7)
C1	0.7405 (3)	0.0970 (2)	0.9777 (4)	0.0613 (9)
H1	0.6790	0.0543	0.9577	0.074*
C2	0.8750 (4)	0.0794 (2)	1.0225 (4)	0.0719 (11)
H2	0.9042	0.0252	1.0326	0.086*
C3	0.9666 (4)	0.1439 (3)	1.0526 (4)	0.0727 (11)
H3	1.0572	0.1324	1.0819	0.087*
C4	0.9246 (4)	0.2231 (3)	1.0396 (4)	0.0715 (11)
H4	0.9865	0.2655	1.0605	0.086*
C5	0.7901 (3)	0.2411 (2)	0.9953 (3)	0.0621 (9)
H5	0.7618	0.2955	0.9876	0.075*
C6	0.6967 (3)	0.17794 (19)	0.9622 (3)	0.0531 (8)
C7	0.5527 (3)	0.19527 (19)	0.9122 (3)	0.0552 (8)
C8	0.3758 (4)	0.28545 (19)	0.8567 (3)	0.0549 (8)
C9	0.3336 (4)	0.36894 (19)	0.8446 (4)	0.0636 (9)
H9	0.3962	0.4106	0.8687	0.076*
C10	0.2031 (4)	0.3884 (2)	0.7983 (3)	0.0640 (10)
H10	0.1771	0.4432	0.7895	0.077*
C11	0.1074 (3)	0.32651 (18)	0.7638 (3)	0.0546 (8)
C12	−0.0303 (4)	0.3392 (2)	0.7114 (3)	0.0659 (10)
H12	−0.0628	0.3924	0.6957	0.079*
C13	−0.1156 (4)	0.2745 (2)	0.6837 (3)	0.0646 (10)
H13	−0.2067	0.2828	0.6516	0.077*
C14	−0.0629 (3)	0.1947 (2)	0.7048 (3)	0.0563 (9)
C15	0.1487 (3)	0.24382 (18)	0.7802 (3)	0.0496 (8)
C16	−0.1497 (3)	0.1216 (2)	0.6737 (3)	0.0572 (8)
C17	−0.2834 (3)	0.1330 (2)	0.6458 (3)	0.0524 (8)
H17	−0.3203	0.1853	0.6456	0.063*

C18	−0.3609 (4)	0.0675 (3)	0.6185 (4)	0.0758 (11)
H18	−0.4535	0.0753	0.6016	0.091*
C19	−0.3142 (4)	−0.0101 (3)	0.6137 (4)	0.0780 (12)
H19	−0.3731	−0.0538	0.5910	0.094*
C20	−0.1784 (4)	−0.0228 (2)	0.6429 (5)	0.0837 (12)
H20	−0.1440	−0.0757	0.6419	0.100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.057 (2)	0.0370 (19)	0.076 (3)	−0.0016 (17)	0.004 (2)	−0.0001 (18)
F1	0.0656 (13)	0.0590 (12)	0.1045 (17)	−0.0053 (10)	0.0094 (12)	0.0308 (11)
F2	0.0820 (14)	0.0531 (12)	0.0938 (16)	0.0081 (10)	0.0004 (12)	−0.0231 (11)
N1	0.0582 (17)	0.0447 (15)	0.0673 (18)	−0.0051 (13)	0.0103 (14)	−0.0005 (13)
N2	0.0567 (16)	0.0411 (14)	0.0544 (16)	−0.0004 (12)	0.0133 (13)	0.0007 (11)
N3	0.0548 (16)	0.0471 (16)	0.0562 (17)	0.0044 (13)	0.0046 (13)	0.0014 (12)
N4	0.087 (2)	0.0626 (16)	0.127 (3)	0.0002 (13)	0.003 (2)	−0.010 (2)
O1	0.0544 (14)	0.0393 (12)	0.1033 (19)	−0.0023 (10)	0.0044 (13)	−0.0031 (12)
C1	0.055 (2)	0.057 (2)	0.072 (2)	−0.0048 (16)	0.0136 (17)	−0.0061 (17)
C2	0.064 (2)	0.069 (2)	0.082 (3)	0.0039 (19)	0.013 (2)	0.001 (2)
C3	0.054 (2)	0.088 (3)	0.078 (3)	−0.003 (2)	0.0167 (18)	0.002 (2)
C4	0.063 (2)	0.079 (3)	0.073 (3)	−0.023 (2)	0.0134 (19)	−0.004 (2)
C5	0.062 (2)	0.058 (2)	0.065 (2)	−0.0068 (17)	0.0100 (17)	0.0013 (17)
C6	0.057 (2)	0.0548 (19)	0.0487 (19)	−0.0083 (16)	0.0122 (15)	−0.0020 (15)
C7	0.064 (2)	0.0468 (18)	0.055 (2)	−0.0083 (16)	0.0139 (16)	−0.0018 (15)
C8	0.072 (2)	0.0411 (17)	0.054 (2)	−0.0048 (16)	0.0174 (17)	0.0001 (14)
C9	0.081 (2)	0.0392 (17)	0.074 (2)	−0.0091 (17)	0.026 (2)	−0.0030 (16)
C10	0.085 (3)	0.0416 (17)	0.070 (2)	0.0082 (18)	0.026 (2)	0.0065 (16)
C11	0.070 (2)	0.0410 (17)	0.054 (2)	0.0042 (16)	0.0153 (17)	0.0020 (14)
C12	0.079 (3)	0.053 (2)	0.067 (2)	0.0212 (19)	0.0168 (19)	0.0050 (17)
C13	0.064 (2)	0.064 (2)	0.064 (2)	0.0207 (19)	0.0080 (18)	0.0035 (18)
C14	0.062 (2)	0.0571 (19)	0.050 (2)	0.0088 (17)	0.0111 (16)	0.0020 (15)
C15	0.0597 (19)	0.0423 (17)	0.0487 (18)	0.0033 (15)	0.0153 (15)	0.0007 (14)
C16	0.0476 (13)	0.0684 (17)	0.0537 (19)	0.0024 (15)	0.0051 (14)	−0.0013 (16)
C17	0.0486 (13)	0.0595 (18)	0.0468 (18)	0.0159 (12)	0.0034 (14)	−0.0014 (14)
C18	0.053 (2)	0.092 (3)	0.078 (3)	−0.0055 (17)	0.0013 (18)	−0.007 (2)
C19	0.064 (3)	0.078 (3)	0.085 (3)	−0.011 (2)	−0.003 (2)	−0.001 (2)
C20	0.072 (3)	0.062 (2)	0.110 (3)	0.0032 (16)	0.001 (2)	−0.001 (2)

Geometric parameters (Å, º)

B1—F1	1.362 (5)	C3—C4	1.355 (6)
B1—F2	1.386 (5)	C4—C5	1.384 (5)
B1—O1	1.472 (5)	C5—C6	1.395 (4)
B1—N2	1.582 (4)	C6—C7	1.480 (5)
N1—C7	1.306 (4)	C8—C9	1.423 (5)
N1—C8	1.368 (4)	C9—C10	1.356 (5)
N2—C8	1.350 (4)	C10—C11	1.396 (5)

N2—C15	1.400 (4)	C11—C15	1.410 (4)
N3—C14	1.325 (4)	C11—C12	1.413 (5)
N3—C15	1.341 (4)	C12—C13	1.358 (5)
N4—C20	1.387 (5)	C13—C14	1.405 (5)
N4—C16	1.400 (5)	C14—C16	1.478 (5)
O1—C7	1.296 (4)	C16—C17	1.344 (4)
C1—C2	1.383 (5)	C17—C18	1.322 (5)
C1—C6	1.390 (5)	C18—C19	1.353 (5)
C2—C3	1.396 (5)	C19—C20	1.367 (5)

F1—B1—F2	112.6 (3)	N2—C8—N1	123.2 (3)
F1—B1—O1	108.5 (3)	N2—C8—C9	119.7 (3)
F2—B1—O1	107.2 (3)	N1—C8—C9	117.1 (3)
F1—B1—N2	110.7 (3)	C10—C9—C8	120.7 (3)
F2—B1—N2	110.0 (3)	C9—C10—C11	120.4 (3)
O1—B1—N2	107.7 (3)	C10—C11—C15	118.8 (3)
C7—N1—C8	119.0 (3)	C10—C11—C12	125.4 (3)
C8—N2—C15	120.3 (3)	C15—C11—C12	115.8 (3)
C8—N2—B1	120.0 (3)	C13—C12—C11	120.7 (3)
C15—N2—B1	119.7 (3)	C12—C13—C14	118.5 (3)
C14—N3—C15	117.8 (3)	N3—C14—C13	123.2 (3)
C20—N4—C16	117.4 (3)	N3—C14—C16	115.6 (3)
C7—O1—B1	125.2 (3)	C13—C14—C16	121.2 (3)
C2—C1—C6	120.4 (3)	N3—C15—N2	115.9 (3)
C1—C2—C3	119.4 (4)	N3—C15—C11	124.0 (3)
C4—C3—C2	120.6 (4)	N2—C15—C11	120.1 (3)
C3—C4—C5	120.3 (4)	C17—C16—N4	122.0 (3)
C4—C5—C6	120.3 (3)	C17—C16—C14	118.0 (3)
C1—C6—C5	118.9 (3)	N4—C16—C14	120.0 (3)
C1—C6—C7	119.5 (3)	C18—C17—C16	117.9 (3)
C5—C6—C7	121.5 (3)	C17—C18—C19	124.2 (4)
O1—C7—N1	125.0 (3)	C18—C19—C20	118.5 (4)
O1—C7—C6	115.0 (3)	C19—C20—N4	119.9 (4)
N1—C7—C6	120.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···F2^{i}	0.93	2.47	3.353 (4)	160

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