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## Structure Reports

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## 2,2-Difluoro-4-phenyl-1,3,2-dioxaborolo[4,5-c]chromen-5-ium-2-ide

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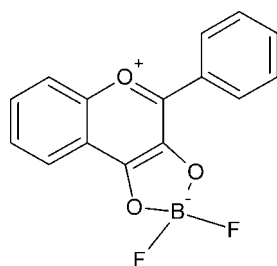
Received 19 November 2010; accepted 23 November 2010

Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.058;  $wR$  factor = 0.234; data-to-parameter ratio = 11.7.

In the crystal, the inversely oriented molecules of the title compound,  $\text{C}_{15}\text{H}_9\text{BF}_2\text{O}_3$ , form stacks along the  $a$  axis via  $\pi-\pi$  interactions between parallel phenylchromenium fragments. Linked by a network of  $\text{C}-\text{H}\cdots\text{F}$  interactions, the stacks form layers in the  $ac$  plane that are dispersively stabilized in the crystal structure. Two F atoms bonded to the B atom are located in the plane perpendicular to the planar skeleton of the molecule made rigid by two intramolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions.

## Related literature

For general background to 3-hydroxy-2-phenyl-4*H*-chromene-4-one (flavonol) and its derivatives, see: Kukhareno & Avramenko (2001); Petković *et al.* (2010); Roshal *et al.* (1998, 2003); Sytnik *et al.* (1994). For related structures, see: Belogh-Hergovich *et al.* (1999); Farina *et al.* (1995); Kaizer *et al.* (2007); Okabe *et al.* (2003). For intermolecular interactions, see: Choudhury & Guru Row (2004); Hunter *et al.* (2001); Novoa *et al.* (2006); Thalladi *et al.* (1998). For the synthesis, see: Roshal *et al.* (2002).



## Experimental

## Crystal data

$\text{C}_{15}\text{H}_9\text{BF}_2\text{O}_3$   
 $M_r = 286.03$   
 Triclinic,  $P\bar{1}$   
 $a = 7.1969$  (10) Å  
 $b = 9.7054$  (11) Å  
 $c = 9.9986$  (15) Å  
 $\alpha = 74.310$  (11)°  
 $\beta = 75.931$  (13)°  
 $\gamma = 71.296$  (11)°  
 $V = 627.43$  (15) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.12$  mm<sup>-1</sup>  
 $T = 295$  K  
 $0.6 \times 0.02 \times 0.02$  mm

## Data collection

Oxford Diffraction Gemini R Ultra Ruby CCD diffractometer  
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)  
 $T_{\min} = 0.945$ ,  $T_{\max} = 0.979$   
 4848 measured reflections  
 2218 independent reflections  
 996 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.034$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$   
 $wR(F^2) = 0.234$   
 $S = 1.10$   
 2218 reflections  
 190 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.24$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}2-\text{H}2\cdots\text{O}3$	0.93	2.37	2.700 (6)	100
$\text{C}6-\text{H}6\cdots\text{O}1$	0.93	2.29	2.967 (6)	129
$\text{C}11-\text{H}11\cdots\text{F}1^i$	0.93	2.44	3.373 (6)	177

Symmetry code: (i)  $-x + 1, -y, -z$ .

Table 2

 $\pi-\pi$  interactions (Å, °).

$\text{Cg}1$ ,  $\text{Cg}2$  and  $\text{Cg}3$  are the centroids of the  $\text{O}3/\text{C}7-\text{C}10/\text{C}15$ ,  $\text{C}10-\text{C}15$  and  $\text{C}1-\text{C}6$  rings, respectively.  $\text{Cg}I\cdots\text{Cg}J$  is the distance between ring centroids. The dihedral angle is that between the planes of the rings  $I$  and  $J$ .  $\text{Cg}I_{\text{Perp}}$  is the perpendicular distance of  $\text{Cg}I$  from ring  $J$ .  $\text{Cg}I_{\text{Offset}}$  is the distance between  $\text{Cg}I$  and the perpendicular projection of  $\text{Cg}J$  on ring  $I$ .

$I$	$J$	$\text{Cg}I\cdots\text{Cg}J$	Dihedral angle	$\text{Cg}I_{\text{Perp}}$	$\text{Cg}I_{\text{Offset}}$
1	1 <sup>ii</sup>	3.512 (3)	0	3.344 (2)	1.076 (2)
1	3 <sup>iii</sup>	3.572 (3)	2.3 (3)	3.450 (2)	0.956 (2)
2	3 <sup>ii</sup>	3.970 (3)	4.3 (3)	3.342 (2)	2.143 (2)
2	3 <sup>iii</sup>	3.925 (3)	4.3 (3)	3.472 (2)	1.831 (2)
3	1 <sup>iii</sup>	3.571 (3)	2.3 (3)	3.428 (2)	1.000 (2)
3	2 <sup>ii</sup>	3.970 (3)	4.3 (3)	3.492 (2)	1.889 (2)
3	2 <sup>iii</sup>	3.925 (3)	4.3 (3)	3.404 (2)	1.954 (2)

Symmetry codes: (ii)  $-x + 1, -y, -z + 1$ ; (iii)  $-x, -y, -z + 1$ .

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5071).

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## supporting information

*Acta Cryst.* (2010). E66, o3354–o3355 [https://doi.org/10.1107/S1600536810048919]

**2,2-Difluoro-4-phenyl-1,3,2-dioxaborolo[4,5-c]chromen-5-ium-2-ide****Michał Wera, Alexander D. Roshal and Jerzy Błażejowski****S1. Comment**

3-Hydroxy-2-phenyl-4*H*-chromene-4-one (flavonol) and its derivatives have been investigated for a long time owing to their unique spectral properties emerging from the excited state intramolecular proton transfer occurring in them (Sytnik *et al.*, 1994). These compounds turned out to be convenient analytical probes because of their considerable ability to complex various chemical entities (molecules, ions) (Roshal *et al.*, 1998; Roshal *et al.*, 2003; Petković *et al.*, 2010). The latter property was the reason for turning our attention to the possibility of applying of flavonol as an analytical spectral probe for boron compounds (Roshal *et al.*, 2002). As part of these investigations we wanted to see how flavonol behaved in the presence of BF<sub>3</sub>. Thus we mixed both reagents in dichloromethane, expecting to obtain a molecular complex of flavonol and BF<sub>3</sub>. The structure of the crystalline product that was actually separated is presented here. It appears that not complexation but condensation of the two reagents, accompanied by the release of HF, takes place (Kukhareenko & Avramenko, 2001) and a molecule of a formally zwitterionic canonical structure was produced. Crystal structures of various flavonol complexes have so far been reported (Farina & Yamin, 1995; Belogh-Hergovich *et al.*, 1999; Okabe *et al.*, 2003; Kaizer *et al.*, 2007), but none of them have contained boron.

The canonical structure of the title compound suggests that the phenylchromenium core of the molecule is aromatic. This is confirmed by analysis of the bond lengths and angles, as well as comparison of the structure determined here with the structures of selected compounds containing flavonol units (Farina *et al.*, 1995; Belogh-Hergovich *et al.*, 1999; Okabe *et al.*, 2003; Kaizer *et al.*, 2007). Furthermore, the average deviation from planarity of the phenylchromenium core is 0.0215 (2) and that of the molecule's skeleton is 0.0373 (2). This implies that both the above-mentioned molecular fragments are planar and that two F atoms at the B atom are located in a plane perpendicular to the molecular one (the dihedral angle between the plane of the molecule's skeleton and the plane of B1–F1–F2 is 89.5 (1)°). Furthermore, two intramolecular C–H···O interactions (Table 1, Fig. 1) stiffen the phenylchromenium core, undoubtedly contributing to its planarity.

In the crystal structure, inversely oriented molecules form stacks along the *a* axis via  $\pi$ - $\pi$  interactions between parallel phenylchromenium fragments (Table 2, Figs. 2 and 3). These stacks are linked by a network of C–H···F interactions arranged in layers in the *ac* plane (Table 1, Figs. 2 and 3). The above-mentioned layers are dispersively stabilized in the crystal lattice. The C–H···O (Novoa *et al.*, 2006) and C–H···F (Thalladi *et al.* (1998); Choudhury & Guru Row (2004)) interactions are of the hydrogen bond type. Like the  $\pi$ - $\pi$  contacts, they are of an attractive nature (Hunter *et al.*, 2001).

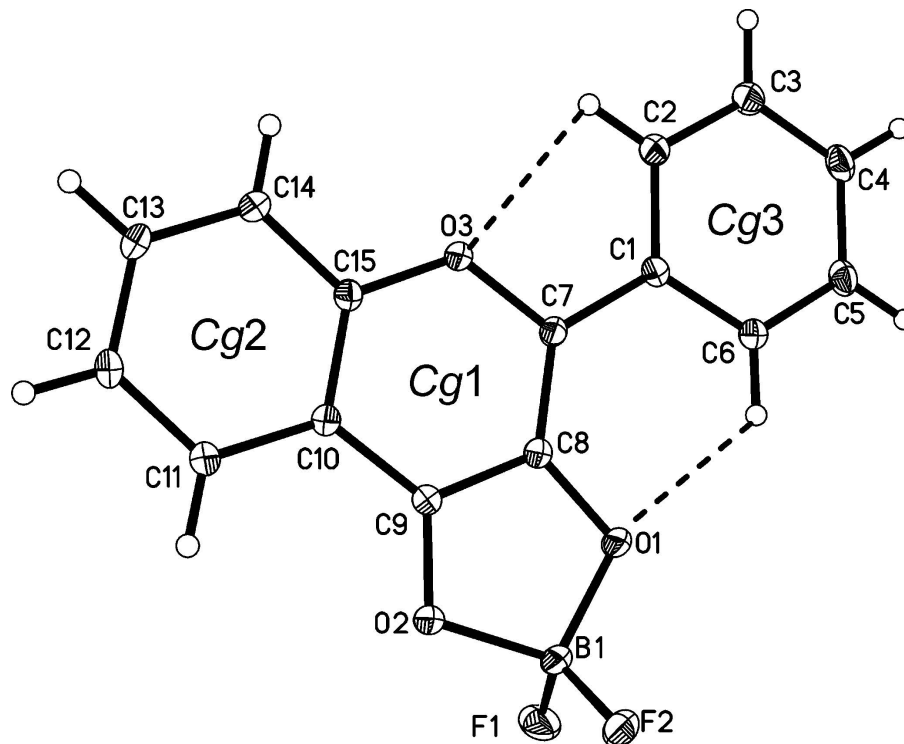
**S2. Experimental**

The title compound was obtained during the reaction of 3-hydroxy-2-phenyl-4*H*-chromene-4-one (flavonol) with BF<sub>3</sub> (Roshal *et al.*, 2002). Thus, boron trifluoride dissolved in anhydrous diethyl ether was added dropwise, with continuous stirring, to an equimolar amount of a saturated solution of flavonol in anhydrous dichloromethane. After evaporation of the solvents, the residue was recrystallized twice from *N,N*-dimethylformamide yielding yellow fluorescing crystals

suitable for X-Ray investigations (m.p. 485 - 487 K).

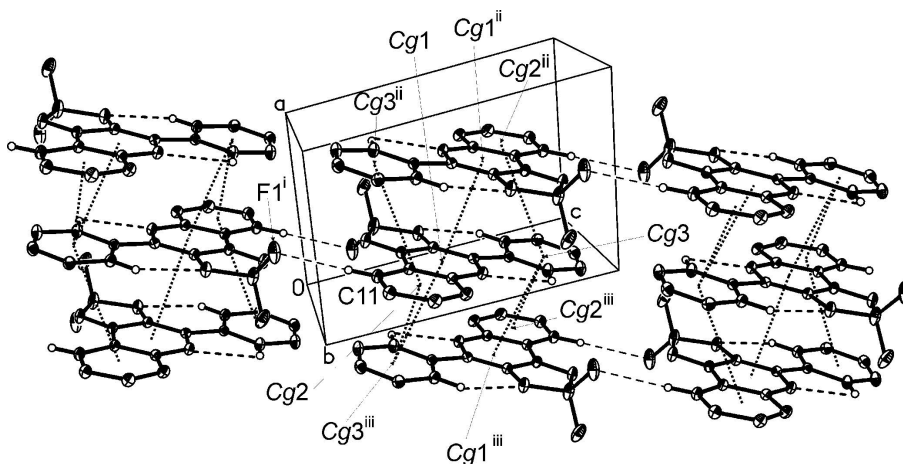
### S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .



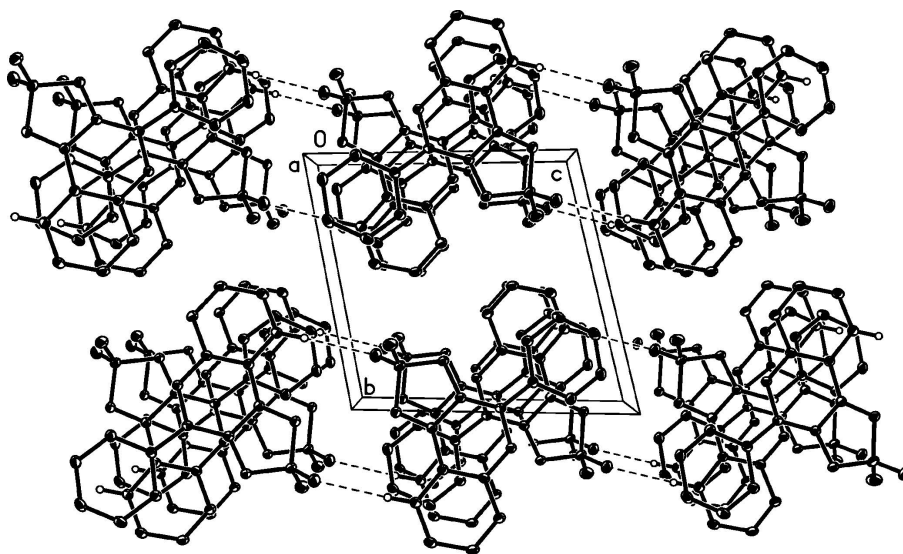
**Figure 1**

The molecular structure of the title compound showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 25% probability level, and H atoms are shown as small spheres of arbitrary radius. *Cg*1, *Cg*2 and *Cg*3 denote the ring centroids. The C—H···O hydrogen bonds are represented by dashed lines.



**Figure 2**

The arrangement of the molecules in the crystal structure. The C–H···O and C–H···F interactions are represented by dashed lines, the  $\pi$ – $\pi$  contacts by dotted lines. H atoms not involved in interactions have been omitted. [Symmetry codes: (i)  $-x + 1, -y, -z$ ; (ii)  $-x + 1, -y, -z + 1$ ; (iii)  $-x, -y, -z + 1$ .]



**Figure 3**

Molecular stacks in the crystal structure, viewed along the  $a$  axis. The C–H···F interactions are represented by dashed lines. H atoms not involved in interactions have been omitted.

### 2,2-Difluoro-4-phenyl-1,3,2-dioxaborolo[4,5-*c*]chromen-5-ium-2-ide

#### Crystal data

$C_{15}H_9BF_2O_3$

$M_r = 286.03$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.1969$  (10) Å

$b = 9.7054$  (11) Å

$c = 9.9986$  (15) Å

$\alpha = 74.310$  (11)°

$\beta = 75.931$  (13)°

$\gamma = 71.296$  (11)°

$V = 627.43$  (15) Å<sup>3</sup>

$Z = 2$

$F(000) = 292$

$D_x = 1.514$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2218 reflections

$\theta = 3.0\text{--}25.1^\circ$   
 $\mu = 0.12\text{ mm}^{-1}$   
 $T = 295\text{ K}$

Needle, yellow  
 $0.6 \times 0.02 \times 0.02\text{ mm}$

#### Data collection

Oxford Diffraction Gemini R Ultra Ruby CCD diffractometer  
 Radiation source: Enhance (Mo) X-ray Source  
 Graphite monochromator  
 Detector resolution:  $10.4002\text{ pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (*CrysAlis RED*; Oxford Diffraction, 2008)  
 $T_{\min} = 0.945$ ,  $T_{\max} = 0.979$

4848 measured reflections  
 2218 independent reflections  
 996 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.034$   
 $\theta_{\max} = 25.1^\circ$ ,  $\theta_{\min} = 3.0^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -10 \rightarrow 11$   
 $l = -9 \rightarrow 11$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.058$   
 $wR(F^2) = 0.234$   
 $S = 1.10$   
 2218 reflections  
 190 parameters  
 0 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0787P)^2 + 0.4107P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.22\text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.24\text{ e \AA}^{-3}$

#### 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.

**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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
B1	0.4867 (13)	-0.1835 (7)	0.2184 (8)	0.075 (2)
O1	0.3873 (5)	-0.2005 (3)	0.3680 (3)	0.0605 (10)
C1	0.1714 (6)	-0.1185 (5)	0.6585 (5)	0.0395 (11)
F1	0.3869 (6)	-0.2186 (4)	0.1401 (3)	0.1025 (14)
O2	0.4773 (5)	-0.0183 (3)	0.1743 (3)	0.0594 (10)
C2	0.0722 (8)	-0.0564 (6)	0.7748 (5)	0.0600 (15)
H2	0.0499	0.0447	0.7694	0.072*
F2	0.6830 (6)	-0.2651 (4)	0.2068 (4)	0.1059 (14)
O3	0.2079 (5)	0.1167 (3)	0.5341 (3)	0.0480 (9)
C3	0.0071 (9)	-0.1459 (6)	0.8983 (6)	0.0680 (16)
H3	-0.0595	-0.1045	0.9764	0.082*
C4	0.0389 (8)	-0.2934 (6)	0.9077 (6)	0.0628 (15)
H4	-0.0061	-0.3521	0.9919	0.075*

C5	0.1364 (8)	-0.3559 (6)	0.7946 (6)	0.0601 (15)
H5	0.1595	-0.4574	0.8022	0.072*
C6	0.2010 (7)	-0.2690 (5)	0.6686 (6)	0.0535 (13)
H6	0.2643	-0.3114	0.5907	0.064*
C7	0.2432 (6)	-0.0265 (5)	0.5263 (5)	0.0408 (11)
C8	0.3379 (7)	-0.0667 (5)	0.3996 (5)	0.0436 (12)
C9	0.3902 (7)	0.0404 (5)	0.2829 (5)	0.0453 (12)
C10	0.3501 (7)	0.1903 (5)	0.2890 (5)	0.0414 (11)
C11	0.3933 (7)	0.3038 (5)	0.1770 (5)	0.0549 (14)
H11	0.4525	0.2835	0.0882	0.066*
C12	0.3484 (8)	0.4446 (6)	0.1983 (6)	0.0587 (14)
H12	0.3739	0.5212	0.1237	0.070*
C13	0.2639 (8)	0.4731 (5)	0.3325 (6)	0.0601 (15)
H13	0.2371	0.5689	0.3466	0.072*
C14	0.2191 (7)	0.3639 (5)	0.4443 (6)	0.0566 (14)
H14	0.1636	0.3844	0.5334	0.068*
C15	0.2586 (7)	0.2227 (5)	0.4210 (5)	0.0454 (12)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
B1	0.113 (6)	0.055 (4)	0.059 (5)	-0.037 (4)	0.023 (4)	-0.031 (4)
O1	0.090 (3)	0.0377 (19)	0.050 (2)	-0.0213 (18)	0.0070 (19)	-0.0153 (16)
C1	0.037 (3)	0.042 (3)	0.039 (3)	-0.013 (2)	-0.005 (2)	-0.007 (2)
F1	0.189 (4)	0.081 (2)	0.059 (2)	-0.073 (3)	0.000 (2)	-0.0260 (19)
O2	0.086 (3)	0.047 (2)	0.041 (2)	-0.0228 (18)	0.0087 (19)	-0.0157 (17)
C2	0.076 (4)	0.058 (3)	0.048 (3)	-0.026 (3)	0.003 (3)	-0.016 (3)
F2	0.122 (3)	0.062 (2)	0.092 (3)	-0.004 (2)	0.040 (2)	-0.025 (2)
O3	0.059 (2)	0.0383 (18)	0.043 (2)	-0.0122 (15)	0.0004 (16)	-0.0117 (16)
C3	0.093 (4)	0.076 (4)	0.037 (3)	-0.036 (3)	0.005 (3)	-0.014 (3)
C4	0.066 (4)	0.073 (4)	0.043 (3)	-0.032 (3)	-0.001 (3)	0.007 (3)
C5	0.058 (3)	0.054 (3)	0.055 (4)	-0.013 (3)	-0.004 (3)	0.003 (3)
C6	0.056 (3)	0.049 (3)	0.054 (3)	-0.016 (3)	-0.002 (3)	-0.012 (3)
C7	0.041 (3)	0.040 (3)	0.041 (3)	-0.009 (2)	-0.006 (2)	-0.010 (2)
C8	0.044 (3)	0.043 (3)	0.039 (3)	-0.009 (2)	-0.004 (2)	-0.008 (2)
C9	0.047 (3)	0.047 (3)	0.041 (3)	-0.014 (2)	0.000 (2)	-0.014 (2)
C10	0.045 (3)	0.038 (3)	0.043 (3)	-0.012 (2)	-0.005 (2)	-0.011 (2)
C11	0.065 (4)	0.050 (3)	0.049 (3)	-0.022 (3)	0.001 (3)	-0.011 (3)
C12	0.066 (4)	0.047 (3)	0.056 (4)	-0.021 (3)	-0.001 (3)	-0.001 (3)
C13	0.071 (4)	0.038 (3)	0.066 (4)	-0.010 (3)	-0.001 (3)	-0.018 (3)
C14	0.062 (3)	0.042 (3)	0.061 (4)	-0.011 (3)	0.001 (3)	-0.018 (3)
C15	0.046 (3)	0.039 (3)	0.046 (3)	-0.012 (2)	-0.002 (2)	-0.006 (2)

*Geometric parameters (Å, °)*

B1—F1	1.349 (8)	C5—C6	1.381 (7)
B1—F2	1.375 (9)	C5—H5	0.9300
B1—O1	1.483 (7)	C6—H6	0.9300

B1—O2	1.527 (7)	C7—C8	1.377 (6)
O1—C8	1.336 (5)	C8—C9	1.402 (6)
C1—C6	1.386 (6)	C9—C10	1.405 (6)
C1—C2	1.387 (6)	C10—C11	1.396 (6)
C1—C7	1.462 (6)	C10—C15	1.395 (6)
O2—C9	1.293 (5)	C11—C12	1.363 (7)
C2—C3	1.378 (7)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.394 (7)
O3—C7	1.351 (5)	C12—H12	0.9300
O3—C15	1.371 (5)	C13—C14	1.371 (7)
C3—C4	1.356 (7)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.380 (6)
C4—C5	1.360 (7)	C14—H14	0.9300
C4—H4	0.9300		
F1—B1—F2	112.0 (5)	O3—C7—C8	117.9 (4)
F1—B1—O1	110.8 (5)	O3—C7—C1	113.2 (4)
F2—B1—O1	110.9 (6)	C8—C7—C1	128.9 (4)
F1—B1—O2	110.6 (6)	O1—C8—C7	128.2 (4)
F2—B1—O2	108.8 (5)	O1—C8—C9	111.7 (4)
O1—B1—O2	103.3 (4)	C7—C8—C9	120.1 (4)
C8—O1—B1	106.4 (4)	O2—C9—C8	111.0 (4)
C6—C1—C2	119.3 (4)	O2—C9—C10	126.5 (4)
C6—C1—C7	120.2 (4)	C8—C9—C10	122.5 (4)
C2—C1—C7	120.6 (4)	C11—C10—C15	119.6 (4)
C9—O2—B1	107.5 (4)	C11—C10—C9	125.9 (5)
C3—C2—C1	119.3 (5)	C15—C10—C9	114.6 (4)
C3—C2—H2	120.3	C12—C11—C10	119.7 (5)
C1—C2—H2	120.3	C12—C11—H11	120.2
C7—O3—C15	122.7 (4)	C10—C11—H11	120.2
C4—C3—C2	120.9 (5)	C11—C12—C13	119.7 (5)
C4—C3—H3	119.5	C11—C12—H12	120.1
C2—C3—H3	119.5	C13—C12—H12	120.1
C3—C4—C5	120.3 (5)	C14—C13—C12	121.9 (5)
C3—C4—H4	119.8	C14—C13—H13	119.1
C5—C4—H4	119.8	C12—C13—H13	119.1
C4—C5—C6	120.2 (5)	C13—C14—C15	118.2 (5)
C4—C5—H5	119.9	C13—C14—H14	120.9
C6—C5—H5	119.9	C15—C14—H14	120.9
C1—C6—C5	119.9 (5)	O3—C15—C14	116.8 (4)
C1—C6—H6	120.1	O3—C15—C10	122.2 (4)
C5—C6—H6	120.1	C14—C15—C10	120.9 (4)
F1—B1—O1—C8	-119.9 (5)	C1—C7—C8—C9	178.1 (4)
F2—B1—O1—C8	114.9 (4)	B1—O2—C9—C8	0.3 (6)
O2—B1—O1—C8	-1.5 (7)	B1—O2—C9—C10	-179.8 (5)
F1—B1—O2—C9	119.3 (5)	O1—C8—C9—O2	-1.4 (6)
F2—B1—O2—C9	-117.2 (5)	C7—C8—C9—O2	-180.0 (4)



O1—B1—O2—C9	0.7 (7)	O1—C8—C9—C10	178.7 (4)
C6—C1—C2—C3	0.7 (7)	C7—C8—C9—C10	0.2 (7)
C7—C1—C2—C3	-179.7 (5)	O2—C9—C10—C11	1.6 (8)
C1—C2—C3—C4	0.1 (8)	C8—C9—C10—C11	-178.5 (5)
C2—C3—C4—C5	0.1 (8)	O2—C9—C10—C15	-178.4 (5)
C3—C4—C5—C6	-1.0 (8)	C8—C9—C10—C15	1.4 (6)
C2—C1—C6—C5	-1.6 (7)	C15—C10—C11—C12	0.9 (7)
C7—C1—C6—C5	178.7 (4)	C9—C10—C11—C12	-179.1 (5)
C4—C5—C6—C1	1.8 (7)	C10—C11—C12—C13	1.5 (8)
C15—O3—C7—C8	1.5 (6)	C11—C12—C13—C14	-1.8 (8)
C15—O3—C7—C1	-178.3 (4)	C12—C13—C14—C15	-0.5 (8)
C6—C1—C7—O3	-178.3 (4)	C7—O3—C15—C14	-178.3 (4)
C2—C1—C7—O3	2.1 (6)	C7—O3—C15—C10	0.2 (7)
C6—C1—C7—C8	1.9 (7)	C13—C14—C15—O3	-178.5 (4)
C2—C1—C7—C8	-177.7 (5)	C13—C14—C15—C10	2.9 (7)
B1—O1—C8—C7	-179.8 (6)	C11—C10—C15—O3	178.3 (4)
B1—O1—C8—C9	1.8 (6)	C9—C10—C15—O3	-1.6 (7)
O3—C7—C8—O1	-179.9 (4)	C11—C10—C15—C14	-3.2 (7)
C1—C7—C8—O1	-0.2 (8)	C9—C10—C15—C14	176.8 (4)
O3—C7—C8—C9	-1.6 (6)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C2—H2 $\cdots$ O3	0.93	2.37	2.700 (6)	100
C6—H6 $\cdots$ O1	0.93	2.29	2.967 (6)	129
C11—H11 $\cdots$ F1 <sup>i</sup>	0.93	2.44	3.373 (6)	177

Symmetry code: (i)  $-x+1, -y, -z$ .