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# 2-[2-(Trifluoromethyl)phenyl]-2*H*-1-benzopyran-4(3*H*)-one

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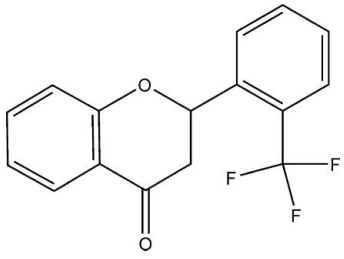
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.087; $wR$ factor = 0.109; data-to-parameter ratio = 13.5.

In the title compound, $C_{16}H_{11}F_3O_2$, the $\gamma$-pyranone ring adopts an envelope conformation with the chiral C atom standing out of the ring plane. In the crystal, molecules are linked by C—H···O and C—H···F interactions.

## Related literature

For general background to flavones, see: Harborne & Williams (2000). For related flavonoids, see: Benavente-García & Castillo (2008); Rodeiro *et al.* (2006). For related structures, see: Wera *et al.* (2012); Białońska *et al.* (2007); Krishnaiah *et al.* (2005); Wu *et al.* (2005). For van der Waals radii, see: Bondi (1964).



## Experimental

### *Crystal data*

$C_{16}H_{11}F_3O_2$
$M_r$ = 292.25
Orthorhombic, $Pna2_1$
$a$ = 8.2291 (9) Å
$b$ = 22.020 (3) Å
$c$ = 7.3355 (11) Å
$V$ = 1329.2 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.12 mm$^{-1}$
$T$ = 293 K
0.18 × 0.02 × 0.02 mm

### *Data collection*

Oxford Diffraction Xcalibur Sapphire3 Gemini diffractometer
4585 measured reflections
2558 independent reflections
1462 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.087
$wR(F^2)$ = 0.109
$S$ = 1.12
2558 reflections
190 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3···O2$^{i}$ | 0.93 | 2.54 | 3.311 (5) | 140 |
| C5—H5···F3$^{ii}$ | 0.93 | 2.54 | 3.313 (5) | 141 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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: *WinGX* (Farrugia, 1999), *PLATON* (Spek, 2009) and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2198).

## References

Benavente-García, O. & Castillo, J. (2008). *J. Agric. Food Chem.* **56**, 6185–6205.
Białońska, A., Ciunik, Z., Kostrzewa-Susłow, E. & Dmochowska-Gładysz, J. (2007). *Acta Cryst.* E**63**, o432–o433.
Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Harborne, J. B. & Williams, C. A. (2000). *Phytochemistry*, **55**, 481–504.
Krishnaiah, M., Ravi Kumar, R., Jagadeesh Kumar, N., Gunasekar, D. & Jayaprakasam, B. (2005). *Acta Cryst.* E**61**, o3565–o3567.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Oxford Diffraction (2010). *CrysAlis PRO*. Oxford Diffraction Ltd., Yarnton, Oxfordshire, England.
Rodeiro, I., Cancino, L., González, J. E., Morffi, J., Garrido, G., González, R. M., Nuñez, A. & Delgado, R. (2006). *Food Chem. Toxicol.* **44**, 1707–1713.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wera, M., Chalyi, A. G., Roshal, A. D. & Błażejowski, J. (2012). *Acta Cryst.* E**68**, o253–o254.
Wu, H., Xu, Z., Wan, Y., Liang, Y.-M. & Yu, K.-B. (2005). *Acta Cryst.* E**61**, o1692–o1693.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o1522 [doi:10.1107/S160053681201687X]

## 2-[2-(Trifluoromethyl)phenyl]-2*H*-1-benzopyran-4(3*H*)-one

**Bojana M. Francuski, Branka Ivković, Ivana Stojanović, Sote Vladimirov and Djordje Francuski**

### Comment

The title compound belongs to the group of flavanones which occur predominantly in citrus fruits. Citrus flavonoids were reported (Benavente-García & Castillo, 2008) as having antimicrobial, antifungal, antiviral, anti–allergenic, anti-inflammatory (Harborne & Williams, 2000) and antioxidant (Rodeiro *et al.*, 2006) properties. Case control studies suggest that flavonoids may reduce the risk of cardiovascular disease and stroke. Considering the wide spectrum of activities of natural flavonoids further structure modification of these molecules is aimed to enhance their interaction with the target sites in cells.

The title compound adopts a typical conformation of flavanones with the *γ*–pyranone ring adopting the envelope conformation. In this conformation the carbon atoms C1, C6, C7, C8 and oxygen O1 are nearly coplanar with a root mean square deviation from the mean plane of 0.035 Å, while the C9 carbon atom is standing out from this plane with an atom–to–plane distance of 0.652 (6) Å. All bond lengths and angles in the title compound show usual values for this type of compounds (Wera *et al.*, 2012; Białońska *et al.*, 2007; Krishnaiah *et al.*, 2005; Wu *et al.*, 2005). In this crystal packing of the title compound there are 4 intramolecular, 2 intermolecular (C—H···O and C—H···F) and one *π*–*π* interaction. All of the fluoride atoms participate in weak intramolecular C—H···F interactions (Fig. 1) with H···F distances equal or shorter than 2.50 Å, which is shorter than the sum of their Van der Waals radii (Bondi, 1964). Two of the fluoride atoms interact with the hydrogen atom connected to the chiral carbon atom C9 while the third fluoride atom interacts with one of the phenyl hydrogen atoms (Table 1). The dihedral angle between *Cg*1 and *Cg*2 rings in previously published structures of flavanones (Wera *et al.*, 2012; Białońska *et al.*, 2007; Krishnaiah *et al.*, 2005; Wu *et al.*, 2005) is in the range from 55 to 75° while the corresponding dihedral angle in the case of the title compound is 66.06 (15)°.

The flavanone molecules are connected into rows by the C3—H3···O2 intermolecular interaction forming chains down the crystallographic *a* axis (Fig. 2). The second intermolecular interaction, C5—H5···F3, connects the molecules into another chain in the direction of the screw axis following the crystallographic *c* axis, thus forming a two dimensional net of molecules (Fig. 3). Strings of molecules along the crystallographic *c* axis are further connected by *π*–*π* interactions (Fig. 4). Perpendicular distance from the centroid of one *Cg*1 ring, molecule at (*x*, *y*, *z*), to the plane of the second *Cg*1 ring, molecule at (1 - *x*, 2 - *y*, 1/2 + *z*), and *vice versa* are 3.70 and 3.62 Å respectively, while the distance between the ring centroids measures 4.101 (3) Å. The *Cg*1 ring planes of molecules at (*x*, *y*, *z*) and (1 - *x*, 2 - *y*, 1/2 + *z*) are nearly parallel with the dihedral angle being 5.59 (3)°.

### Experimental

The proposed compound was prepared in two steps. The first step in the synthetic route consisted of the condensation of 2-hydroxy acetophenone with 2-trifluoromethylbenzaldehyde to give an *α*,*β*-unsaturated ketone (chalcone). In the second step the obtained chalcone was dissolved under stirring in a 50:50 water/ethanol mixture. The pH was set to 9.0 with 0.1 *M* NaOH and the reaction mixture was refluxed for 2 h after which it was cooled over night to room temperature. Small

crystals of the title compound formed in the reaction vessel and, after draining excess fluid, the crystals were dried at room temperature.

### Refinement

The H atoms bonded to C atoms were placed at geometrically calculated positions and refined using a riding model. C—H distances were fixed to 0.93 Å for aromatic C atoms, 0.97 Å for the secondary $CH_2$ group and 0.98 Å for the tertiary CH group. Their $U_{iso}$(H) values were equal to 1.2 times $U_{eq}$ of the corresponding C atom.

In the absence of significant anomalous scattering, the absolute configuration could not be reliably determined so the Friedel pairs were merged and any references to the Flack parameter were removed.

### Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010); 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: *WinGX* (Farrugia, 1999), *PLATON* (Spek, 2009) and *PARST* (Nardelli, 1995).

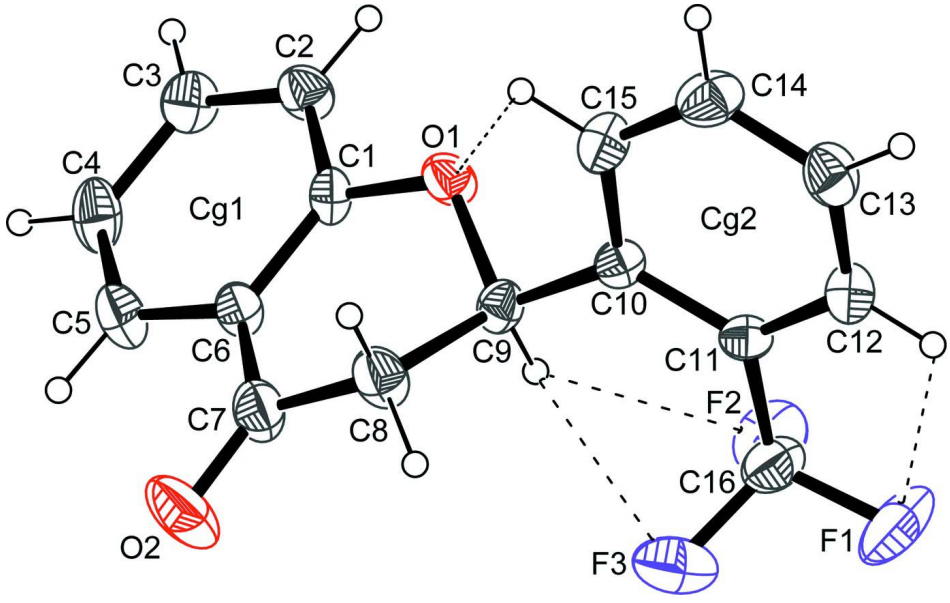


**Figure 1**

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non–H atoms. H atoms are represented as small spheres of arbitrary radii. Intramolecular interactions are shown as dashed lines.

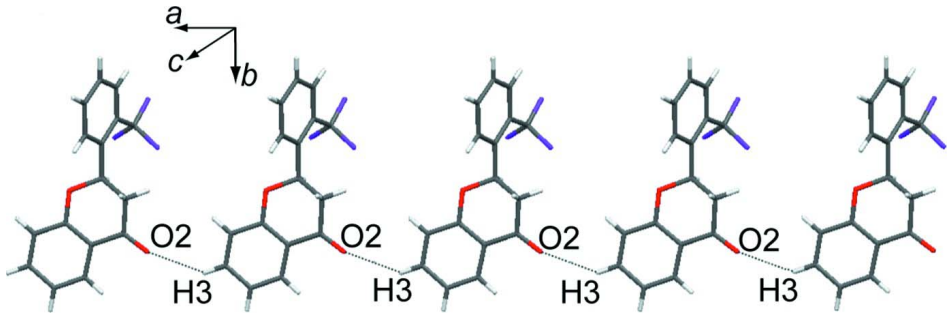


**Figure 2**

Molecular packing of the title compound and intermolecular interactions along the crystallographic *a* axis.

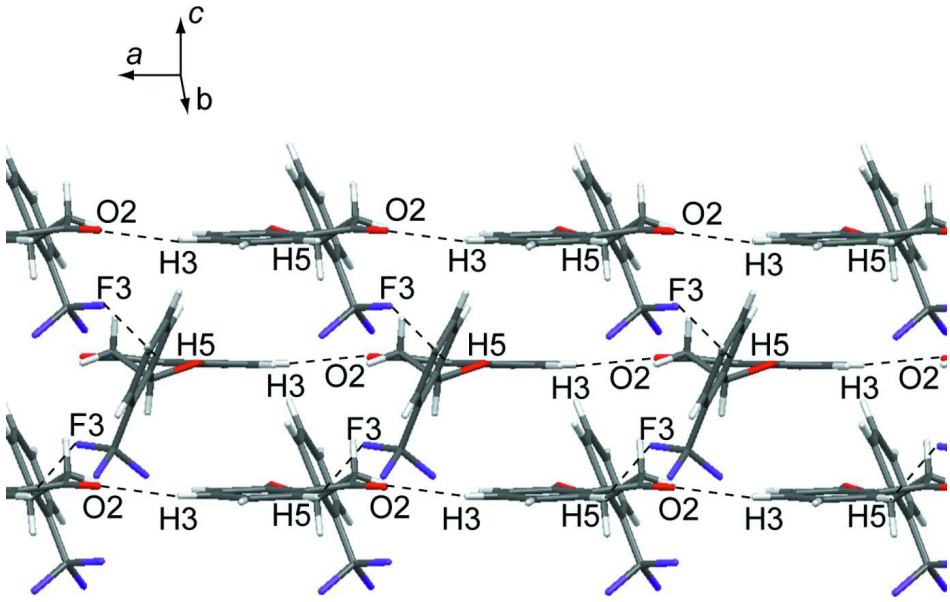


**Figure 3**

Molecular packing of the title compound and intermolecular interactions along the crystallographic *c* axis.

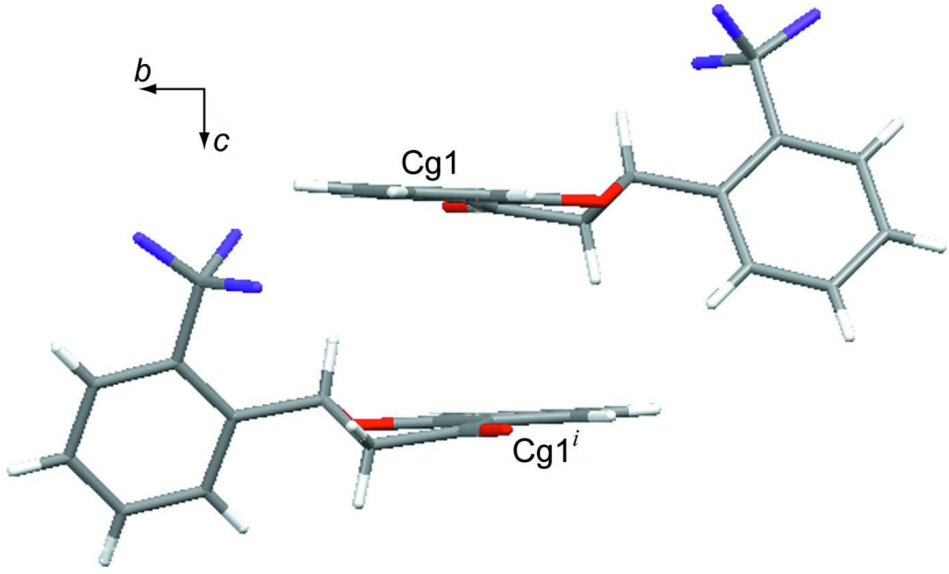


**Figure 4**

$\pi$–$\pi$ interactions of two neighbouring *Cg*1 rings. Symmetry code: (*i*) 1 - *x*, 2 - *y*, 1/2 + *z*.

### 2-[2-(Trifluoromethyl)phenyl]-2*H*-1-benzopyran-4(3*H*)-one

*Crystal data*

$C_{16}H_{11}F_3O_2$
$M_r$ = 292.25
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a$ = 8.2291 (9) Å
$b$ = 22.020 (3) Å
$c$ = 7.3355 (11) Å
$V$ = 1329.2 (3) Å$^3$
$Z$ = 4
$F(000)$ = 600
$D_x$ = 1.460 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 966 reflections
$\theta$ = 3.3–28.9°
$\mu$ = 0.12 mm$^{-1}$
$T$ = 293 K
Needle, colourless
0.18 × 0.02 × 0.02 mm

*Data collection*

Oxford Diffraction Xcalibur Sapphire3 Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.3280 pixels mm$^{-1}$
$\omega$ scans
4585 measured reflections
2558 independent reflections
1462 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049
$\theta_{max}$ = 28.9°, $\theta_{min}$ = 3.7°
$h$ = −11→10
$k$ = −28→29
$l$ = −9→9

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.087
$wR(F^2)$ = 0.109
$S$ = 1.12
2558 reflections
190 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.025P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 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.

**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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.3661 (3) | 0.90660 (11) | 0.7245 (5) | 0.0481 (8) |
| O2 | −0.0253 (3) | 1.02162 (14) | 0.7338 (6) | 0.0901 (14) |
| F1 | 0.0147 (4) | 0.74844 (13) | 0.3065 (5) | 0.1002 (11) |
| F2 | 0.1886 (3) | 0.82036 (13) | 0.2974 (4) | 0.0759 (8) |
| F3 | −0.0440 (3) | 0.83559 (15) | 0.4155 (5) | 0.0867 (10) |
| C1 | 0.3889 (4) | 0.96841 (17) | 0.7160 (7) | 0.0394 (10) |
| C2 | 0.5488 (4) | 0.98855 (19) | 0.7098 (7) | 0.0475 (12) |
| H2 | 0.6339 | 0.9608 | 0.7105 | 0.057* |
| C3 | 0.5801 (5) | 1.04910 (19) | 0.7029 (7) | 0.0496 (12) |
| H3 | 0.6872 | 1.0626 | 0.7023 | 0.060* |
| C4 | 0.4543 (5) | 1.09121 (19) | 0.6967 (7) | 0.0581 (13) |
| H4 | 0.4767 | 1.1325 | 0.6878 | 0.070* |
| C5 | 0.2973 (5) | 1.07110 (18) | 0.7040 (7) | 0.0557 (13) |
| H5 | 0.2132 | 1.0993 | 0.7028 | 0.067* |
| C6 | 0.2595 (4) | 1.00912 (18) | 0.7131 (7) | 0.0416 (11) |
| C7 | 0.0917 (5) | 0.98787 (19) | 0.7367 (8) | 0.0563 (14) |
| C8 | 0.0756 (4) | 0.92045 (17) | 0.7675 (7) | 0.0555 (15) |
| H8A | −0.0302 | 0.9070 | 0.7254 | 0.067* |
| H8B | 0.0831 | 0.9119 | 0.8969 | 0.067* |
| C9 | 0.2082 (4) | 0.88567 (18) | 0.6662 (6) | 0.0393 (11) |
| H9 | 0.1964 | 0.8925 | 0.5349 | 0.047* |
| C10 | 0.2017 (4) | 0.81852 (19) | 0.7043 (6) | 0.0365 (10) |
| C11 | 0.1381 (5) | 0.7759 (2) | 0.5836 (6) | 0.0387 (11) |
| C12 | 0.1326 (5) | 0.7148 (2) | 0.6313 (7) | 0.0478 (13) |
| H12 | 0.0877 | 0.6868 | 0.5509 | 0.057* |
| C13 | 0.1925 (5) | 0.6955 (2) | 0.7952 (8) | 0.0540 (12) |
| H13 | 0.1884 | 0.6545 | 0.8253 | 0.065* |
| C14 | 0.2581 (5) | 0.7360 (2) | 0.9145 (7) | 0.0583 (14) |
| H14 | 0.2998 | 0.7227 | 1.0254 | 0.070* |
| C15 | 0.2626 (5) | 0.7976 (2) | 0.8697 (7) | 0.0505 (13) |
| H15 | 0.3071 | 0.8252 | 0.9518 | 0.061* |
| C16 | 0.0756 (6) | 0.7942 (2) | 0.4026 (8) | 0.0594 (15) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0319 (14) | 0.0360 (17) | 0.076 (2) | −0.0008 (13) | −0.0020 (16) | 0.001 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O2 | 0.0468 (16) | 0.064 (2) | 0.160 (4) | 0.0188 (17) | 0.013 (2) | 0.002 (3) |
| F1 | 0.149 (3) | 0.079 (2) | 0.072 (2) | −0.041 (2) | −0.051 (2) | −0.002 (2) |
| F2 | 0.0938 (18) | 0.087 (2) | 0.0464 (17) | −0.0169 (17) | 0.0070 (17) | 0.0086 (19) |
| F3 | 0.0697 (18) | 0.097 (2) | 0.093 (2) | 0.0126 (19) | −0.0212 (18) | 0.022 (2) |
| C1 | 0.044 (2) | 0.032 (2) | 0.042 (3) | −0.002 (2) | 0.007 (2) | −0.009 (3) |
| C2 | 0.035 (2) | 0.046 (3) | 0.062 (3) | 0.000 (2) | 0.007 (3) | 0.001 (3) |
| C3 | 0.050 (2) | 0.045 (3) | 0.055 (3) | −0.011 (2) | 0.006 (3) | 0.005 (3) |
| C4 | 0.070 (3) | 0.031 (2) | 0.073 (4) | −0.011 (3) | 0.018 (3) | −0.005 (3) |
| C5 | 0.060 (3) | 0.036 (3) | 0.071 (3) | 0.009 (2) | 0.010 (3) | −0.001 (3) |
| C6 | 0.041 (2) | 0.036 (3) | 0.049 (3) | 0.002 (2) | 0.005 (3) | −0.002 (3) |
| C7 | 0.047 (2) | 0.047 (3) | 0.076 (4) | 0.002 (2) | 0.006 (3) | −0.013 (4) |
| C8 | 0.037 (2) | 0.045 (3) | 0.085 (4) | −0.002 (2) | 0.009 (3) | −0.004 (3) |
| C9 | 0.040 (2) | 0.042 (2) | 0.036 (3) | −0.003 (2) | 0.005 (2) | −0.007 (2) |
| C10 | 0.0344 (19) | 0.037 (3) | 0.038 (3) | −0.005 (2) | 0.001 (2) | 0.002 (3) |
| C11 | 0.030 (2) | 0.044 (3) | 0.042 (3) | −0.001 (2) | −0.002 (2) | 0.002 (3) |
| C12 | 0.056 (3) | 0.041 (3) | 0.046 (3) | −0.001 (3) | 0.004 (2) | −0.005 (3) |
| C13 | 0.060 (3) | 0.035 (3) | 0.067 (3) | −0.004 (3) | 0.005 (3) | 0.006 (3) |
| C14 | 0.066 (3) | 0.060 (4) | 0.050 (3) | −0.009 (3) | −0.014 (3) | 0.015 (3) |
| C15 | 0.061 (3) | 0.046 (3) | 0.045 (3) | −0.008 (2) | −0.001 (3) | −0.006 (3) |
| C16 | 0.060 (3) | 0.058 (4) | 0.060 (4) | −0.011 (3) | −0.016 (3) | 0.001 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.376 (4) | C7—C8 | 1.508 (5) |
| O1—C9 | 1.443 (4) | C8—C9 | 1.526 (5) |
| O2—C7 | 1.217 (4) | C8—H8A | 0.9700 |
| F1—C16 | 1.328 (5) | C8—H8B | 0.9700 |
| F2—C16 | 1.339 (5) | C9—C10 | 1.506 (5) |
| F3—C16 | 1.345 (5) | C9—H9 | 0.9800 |
| C1—C2 | 1.389 (5) | C10—C15 | 1.391 (5) |
| C1—C6 | 1.392 (5) | C10—C11 | 1.392 (5) |
| C2—C3 | 1.359 (5) | C11—C12 | 1.390 (6) |
| C2—H2 | 0.9300 | C11—C16 | 1.480 (7) |
| C3—C4 | 1.390 (5) | C12—C13 | 1.367 (6) |
| C3—H3 | 0.9300 | C12—H12 | 0.9300 |
| C4—C5 | 1.367 (5) | C13—C14 | 1.361 (6) |
| C4—H4 | 0.9300 | C13—H13 | 0.9300 |
| C5—C6 | 1.401 (5) | C14—C15 | 1.397 (6) |
| C5—H5 | 0.9300 | C14—H14 | 0.9300 |
| C6—C7 | 1.468 (5) | C15—H15 | 0.9300 |
| | | | |
| C1—O1—C9 | 115.2 (3) | O1—C9—C8 | 109.8 (3) |
| O1—C1—C2 | 116.5 (3) | C10—C9—C8 | 112.2 (3) |
| O1—C1—C6 | 122.3 (3) | O1—C9—H9 | 109.3 |
| C2—C1—C6 | 121.2 (3) | C10—C9—H9 | 109.3 |
| C3—C2—C1 | 119.6 (4) | C8—C9—H9 | 109.3 |
| C3—C2—H2 | 120.2 | C15—C10—C11 | 117.9 (4) |
| C1—C2—H2 | 120.2 | C15—C10—C9 | 118.3 (4) |
| C2—C3—C4 | 121.0 (4) | C11—C10—C9 | 123.9 (4) |
| C2—C3—H3 | 119.5 | C12—C11—C10 | 120.3 (4) |

| | | | |
|---|---|---|---|
| C4—C3—H3 | 119.5 | C12—C11—C16 | 118.5 (4) |
| C5—C4—C3 | 119.1 (4) | C10—C11—C16 | 121.2 (4) |
| C5—C4—H4 | 120.4 | C13—C12—C11 | 120.7 (5) |
| C3—C4—H4 | 120.4 | C13—C12—H12 | 119.7 |
| C4—C5—C6 | 121.8 (4) | C11—C12—H12 | 119.7 |
| C4—C5—H5 | 119.1 | C14—C13—C12 | 120.3 (5) |
| C6—C5—H5 | 119.1 | C14—C13—H13 | 119.8 |
| C1—C6—C5 | 117.3 (3) | C12—C13—H13 | 119.8 |
| C1—C6—C7 | 120.8 (4) | C13—C14—C15 | 119.7 (5) |
| C5—C6—C7 | 121.6 (4) | C13—C14—H14 | 120.1 |
| O2—C7—C6 | 123.2 (4) | C15—C14—H14 | 120.1 |
| O2—C7—C8 | 122.3 (4) | C10—C15—C14 | 121.1 (4) |
| C6—C7—C8 | 114.5 (4) | C10—C15—H15 | 119.4 |
| C7—C8—C9 | 111.0 (3) | C14—C15—H15 | 119.4 |
| C7—C8—H8A | 109.4 | F1—C16—F2 | 106.4 (5) |
| C9—C8—H8A | 109.4 | F1—C16—F3 | 106.0 (4) |
| C7—C8—H8B | 109.4 | F2—C16—F3 | 104.9 (4) |
| C9—C8—H8B | 109.4 | F1—C16—C11 | 113.7 (4) |
| H8A—C8—H8B | 108.0 | F2—C16—C11 | 113.2 (4) |
| O1—C9—C10 | 106.9 (3) | F3—C16—C11 | 112.0 (5) |
| | | | |
| C9—O1—C1—C2 | −158.8 (4) | C7—C8—C9—C10 | 176.3 (4) |
| C9—O1—C1—C6 | 21.0 (7) | O1—C9—C10—C15 | 43.2 (5) |
| O1—C1—C2—C3 | −179.4 (5) | C8—C9—C10—C15 | −77.3 (5) |
| C6—C1—C2—C3 | 0.7 (8) | O1—C9—C10—C11 | −136.9 (4) |
| C1—C2—C3—C4 | −1.8 (8) | C8—C9—C10—C11 | 102.7 (4) |
| C2—C3—C4—C5 | 2.2 (8) | C15—C10—C11—C12 | 1.7 (6) |
| C3—C4—C5—C6 | −1.6 (8) | C9—C10—C11—C12 | −178.2 (4) |
| O1—C1—C6—C5 | −179.9 (4) | C15—C10—C11—C16 | −178.1 (4) |
| C2—C1—C6—C5 | −0.1 (7) | C9—C10—C11—C16 | 2.0 (6) |
| O1—C1—C6—C7 | 5.9 (7) | C10—C11—C12—C13 | −1.4 (6) |
| C2—C1—C6—C7 | −174.3 (5) | C16—C11—C12—C13 | 178.4 (4) |
| C4—C5—C6—C1 | 0.5 (8) | C11—C12—C13—C14 | 0.2 (7) |
| C4—C5—C6—C7 | 174.7 (5) | C12—C13—C14—C15 | 0.7 (7) |
| C1—C6—C7—O2 | −179.4 (6) | C11—C10—C15—C14 | −0.9 (6) |
| C5—C6—C7—O2 | 6.6 (9) | C9—C10—C15—C14 | 179.1 (4) |
| C1—C6—C7—C8 | 1.3 (7) | C13—C14—C15—C10 | −0.3 (7) |
| C5—C6—C7—C8 | −172.6 (5) | C12—C11—C16—F1 | 2.2 (7) |
| O2—C7—C8—C9 | 148.5 (5) | C10—C11—C16—F1 | −178.0 (4) |
| C6—C7—C8—C9 | −32.3 (6) | C12—C11—C16—F2 | −119.4 (4) |
| C1—O1—C9—C10 | −174.2 (4) | C10—C11—C16—F2 | 60.4 (6) |
| C1—O1—C9—C8 | −52.2 (5) | C12—C11—C16—F3 | 122.3 (4) |
| C7—C8—C9—O1 | 57.6 (5) | C10—C11—C16—F3 | −57.9 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9···F2 | 0.98 | 2.36 | 3.068 (5) | 129 |
| C9—H9···F3 | 0.98 | 2.50 | 2.984 (5) | 110 |

| | | | | |
|---|---|---|---|---|
| C12—H12···F1 | 0.93 | 2.33 | 2.677 (6) | 102 |
| C15—H15···O1 | 0.93 | 2.50 | 2.760 (5) | 96 |
| C3—H3···O2$^{i}$ | 0.93 | 2.54 | 3.311 (5) | 140 |
| C5—H5···F3$^{ii}$ | 0.93 | 2.54 | 3.313 (5) | 141 |

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, -y+2, z+1/2$.