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# 6-Fluoro-4-oxo-4*H*-chromene-3-carbaldehyde

**Yoshinobu Ishikawa**

School of Pharmaceutical Sciences, University of Shizuoka, 52-1 Yada, Suruga-ku, Shizuoka 422-8526, Japan
Correspondence e-mail: ishi206@u-shizuoka-ken.ac.jp

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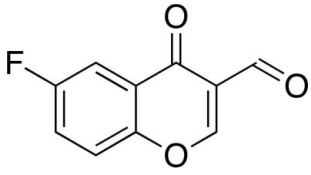
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.106; data-to-parameter ratio = 14.2.

In the title compound, $C_{10}H_5FO_3$, the non-H atoms are essentially coplanar (r.m.s. deviation = 0.0071 Å), with the largest deviation from the mean plane [0.0203 (15) Å] being found for the ring C atom in the 2-position. In the crystal, molecules are linked into a three-dimensional architecture *via* C—H···O hydrogen bonds and $\pi$–$\pi$ stacking interactions between the chromone units along the *a*-axis direction [centroid–centroid distance between the benzene and pyran rings = 3.707 (2) Å].

## Related literature

For related structures, see: Ishikawa (2014*a*,*b*). For halogen bonding, see: Auffinger *et al.* (2004); Metrangolo *et al.* (2005); Wilcken *et al.* (2013); Sirimulla *et al.* (2013).




## Experimental

### Crystal data

$C_{10}H_5FO_3$
$M_r$ = 192.15
Monoclinic, $P2_1/n$
$a$ = 7.8530 (19) Å
$b$ = 5.6020 (17) Å
$c$ = 17.987 (5) Å
$\beta$ = 95.09 (2)°
$V$ = 788.2 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.14 mm$^{-1}$
$T$ = 100 K
0.30 × 0.20 × 0.12 mm

### Data collection

Rigaku AFC-7R diffractometer
2412 measured reflections
1815 independent reflections
1496 reflections with $F^2 > 2\sigma(F^2)$
$R_{int}$ = 0.024
3 standard reflections every 150 reflections
intensity decay: 3.4%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.106
$S$ = 1.03
1815 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O3$^{i}$ | 0.95 | 2.37 | 3.308 (2) | 171 |
| C4—H2···O2$^{ii}$ | 0.95 | 2.35 | 3.235 (2) | 154 |
| C6—H3···O3$^{iii}$ | 0.95 | 2.48 | 3.198 (2) | 133 |

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

Data collection: *WinAFC Diffractometer Control Software* (Rigaku, 1999); cell refinement: *WinAFC Diffractometer Control Software*; data reduction: *WinAFC Diffractometer Control Software*; program(s) used to solve structure: *SIR2008* (Burla *et al.*, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *CrystalStructure*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5307).

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# supporting information

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## 6-Fluoro-4-oxo-4*H*-chromene-3-carbaldehyde

**Yoshinobu Ishikawa**

### S1. Structural commentary

Halogen bonds have been found to occur in organic, inorganic and biological systems, and have recently attracted much attention in medicinal chemistry, chemical biology and supramolecular chemistry (Auffinger *et al.*, 2004, Metrangolo *et al.*, 2005, Wilcken *et al.*, 2013, Sirimulla *et al.*, 2013). We have recently reported the crystal structures of monohalogenated 3-formylchromone derivatives 6-bromo-4-oxo-4*H*-chromene-3-carbaldehyde (Ishikawa, 2014*a*) and 6-chloro-4-oxo-4*H*-chromene-3-carbaldehyde (Ishikawa, 2014*b*). Halogen bonding is observed in the former, but is not observed in the latter. As part of our interest in this type of chemical bonding, we herein report the crystal structure of a monofluorinated 3-formylchromone derivative, 6-fluoro-4-oxo-4*H*-chromene-3-carbaldehyde. The objective of this study is to reveal whether halogen bond(*s*) can be formed in the crystal structure of this compound with a fluorine atom at the 6-position.

The mean deviation of the least-square planes for the non-hydrogen atoms is 0.0071 Å, and the largest deviation is 0.0203 (15) Å for C1 (Fig. 1). This mean that the atoms are essentially coplanar. In the crystal, the molecules are linked *via* C—H···O hydrogen bonds and are further linked by $\pi$—$\pi$ stacking interactions between the chromone units [centroid–centroid distance between the benzene and pyran rings = 3.707 (2) Å], into a three-dimensional architectureFig. 1. The distance between the fluorine and proximal formyl oxygen atoms [3.498 (2) Å, Fig.2 (bottom)] is far from halogen bonding. The fact that halogen bonding is observed in the crystal structure of 6-bromo-4-oxo-4*H*-chromene-3-carbaldehyde (Fig. 2 (top)) but is not observed in those of 6-chloro-4-oxo-4*H*-chromene-3-carbaldehyde (Fig. 2 (middle)) and the title compound demonstrates the trend of the size of $\sigma$-hole on halogens (Br > Cl > F; Sirimulla *et al.*, 2013).

### S2. Synthesis and crystallization

Single crystals suitable for X-ray diffraction were obtained by slow evaporation at room temperature of an ethyl acetate solution of the commercially available title compound.

### S3. Refinement

The C($sp^2$)-bound hydrogen atoms were placed in geometrical positions [C—H = 0.95 Å, $U_{iso}$(H) = 1.2$U_{eq}$(C)], and refined using a riding model. One reflection (0 1 1) was omitted because of systematic error.

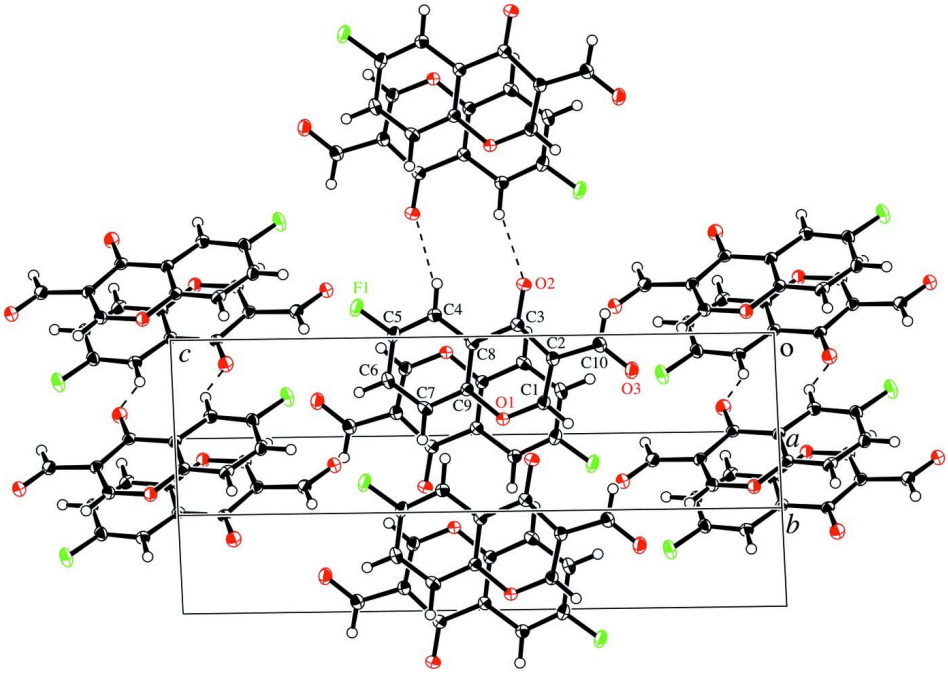


**Figure 1**

A packing view of the title compound with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms are shown as small spheres of arbitrary radius. The shortest intermolecular C—H···O hydrogen bonds are represented as dashed lines.

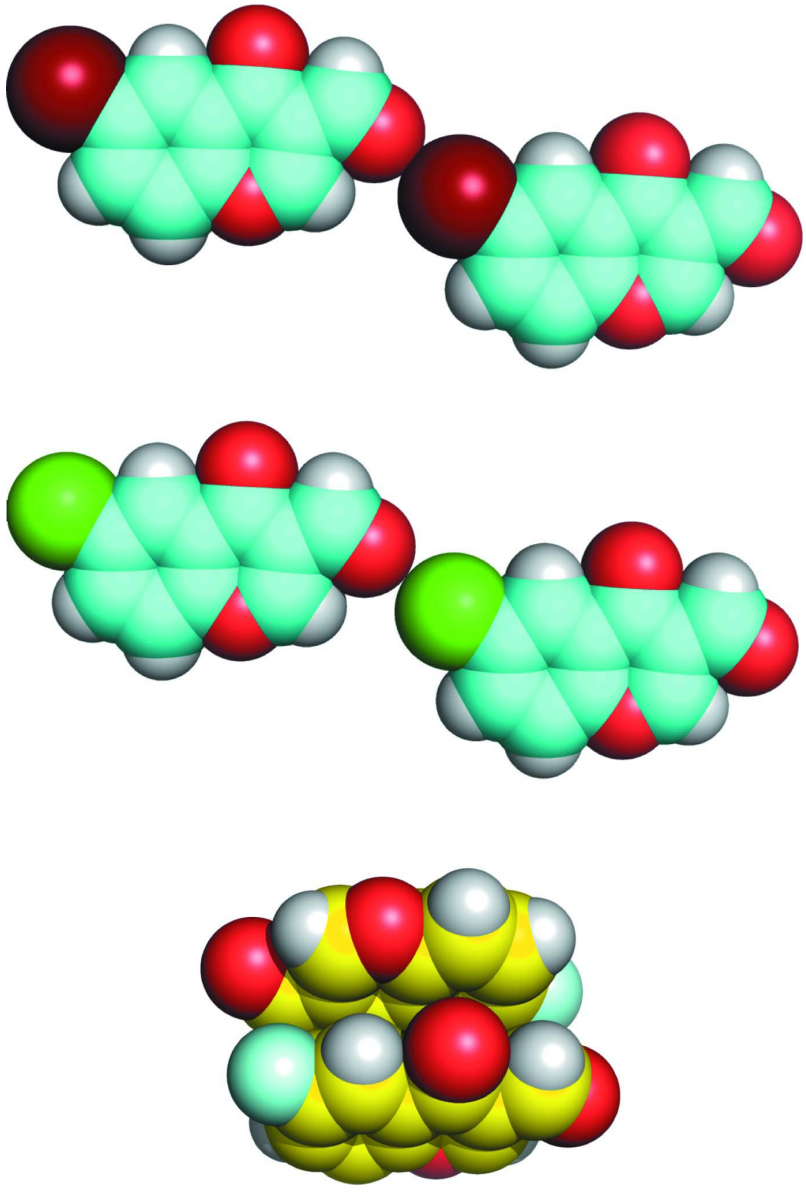

**Figure 2**

Sphere models of the crystal structures of 6-bromo-4-oxo-4*H*-chromene-3-carbaldehyde (top), 6-chloro-4-oxo-4*H*-chromene-3-carbaldehyde (middle), and the title compound (bottom).

### 6-Fluoro-4-oxo-4*H*-chromene-3-carbaldehyde

*Crystal data*

$C_{10}H_5FO_3$
$M_r = 192.15$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.8530$ (19) Å
$b = 5.6020$ (17) Å
$c = 17.987$ (5) Å
$\beta = 95.09$ (2)°
$V = 788.2$ (4) Å$^3$
$Z = 4$
$F(000) = 392.00$
$D_x = 1.619$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 15.2$–17.3°
$\mu = 0.14$ mm$^{-1}$

$T$ = 100 K
Plate, colourless

0.30 × 0.20 × 0.12 mm

*Data collection*

Rigaku AFC-7R diffractometer
$\omega$–$2\theta$ scans
2412 measured reflections
1815 independent reflections
1496 reflections with $F^2 > 2\sigma(F^2)$
$R_{int}$ = 0.024

$\theta_{max}$ = 27.5°
$h$ = −10→10
$k$ = −4→7
$l$ = −23→13
3 standard reflections every 150 reflections
intensity decay: 3.4%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.106
$S$ = 1.03
1815 reflections
128 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
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.3686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008)
Extinction coefficient: 0.011 (3)

*Special details*

**Refinement**. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on $F^2$. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 0.24629 (11) | −0.31171 (17) | 0.68919 (5) | 0.0261 (3) |
| O1 | 0.33585 (12) | 0.28450 (17) | 0.45542 (5) | 0.0178 (3) |
| O2 | 0.05794 (13) | −0.32557 (18) | 0.41030 (5) | 0.0205 (3) |
| O3 | 0.13190 (13) | 0.13025 (19) | 0.23839 (5) | 0.0226 (3) |
| C1 | 0.26630 (17) | 0.2332 (3) | 0.38638 (8) | 0.0169 (3) |
| C2 | 0.17422 (16) | 0.0346 (3) | 0.36799 (7) | 0.0155 (3) |
| C3 | 0.14094 (16) | −0.1427 (3) | 0.42424 (7) | 0.0147 (3) |
| C4 | 0.19425 (16) | −0.2340 (3) | 0.56069 (7) | 0.0163 (3) |
| C5 | 0.26679 (17) | −0.1674 (3) | 0.62980 (7) | 0.0185 (3) |
| C6 | 0.36078 (17) | 0.0417 (3) | 0.64257 (8) | 0.0191 (3) |
| C7 | 0.38313 (17) | 0.1905 (3) | 0.58328 (8) | 0.0182 (3) |
| C8 | 0.21614 (16) | −0.0827 (3) | 0.50018 (7) | 0.0142 (3) |
| C9 | 0.30989 (16) | 0.1270 (3) | 0.51258 (7) | 0.0147 (3) |
| C10 | 0.10652 (17) | −0.0034 (3) | 0.28948 (7) | 0.0187 (3) |
| H1 | 0.2830 | 0.3442 | 0.3478 | 0.0203* |
| H2 | 0.1311 | −0.3782 | 0.5541 | 0.0195* |
| H3 | 0.4087 | 0.0810 | 0.6914 | 0.0229* |
| H4 | 0.4472 | 0.3338 | 0.5904 | 0.0218* |
| H5 | 0.0388 | −0.1414 | 0.2783 | 0.0224* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0315 (5) | 0.0312 (5) | 0.0153 (5) | −0.0033 (4) | 0.0012 (4) | 0.0069 (4) |
| O1 | 0.0222 (5) | 0.0154 (5) | 0.0157 (5) | −0.0035 (4) | 0.0014 (4) | 0.0000 (4) |
| O2 | 0.0223 (5) | 0.0183 (5) | 0.0204 (5) | −0.0056 (4) | −0.0003 (4) | −0.0014 (4) |
| O3 | 0.0293 (6) | 0.0222 (6) | 0.0161 (5) | 0.0045 (5) | 0.0013 (4) | 0.0016 (4) |
| C1 | 0.0186 (7) | 0.0171 (7) | 0.0153 (6) | 0.0018 (5) | 0.0033 (5) | 0.0010 (5) |
| C2 | 0.0146 (6) | 0.0166 (7) | 0.0154 (7) | 0.0024 (5) | 0.0026 (5) | −0.0014 (5) |
| C3 | 0.0125 (6) | 0.0151 (6) | 0.0167 (7) | 0.0024 (5) | 0.0021 (5) | −0.0014 (5) |
| C4 | 0.0149 (6) | 0.0163 (7) | 0.0178 (7) | 0.0001 (5) | 0.0029 (5) | −0.0001 (6) |
| C5 | 0.0192 (7) | 0.0215 (7) | 0.0152 (7) | 0.0032 (6) | 0.0042 (5) | 0.0033 (6) |
| C6 | 0.0177 (6) | 0.0246 (8) | 0.0147 (6) | 0.0027 (6) | −0.0003 (5) | −0.0034 (6) |
| C7 | 0.0163 (7) | 0.0177 (7) | 0.0204 (7) | 0.0002 (5) | 0.0010 (5) | −0.0051 (6) |
| C8 | 0.0120 (6) | 0.0154 (6) | 0.0154 (7) | 0.0019 (5) | 0.0023 (5) | −0.0015 (5) |
| C9 | 0.0146 (6) | 0.0151 (7) | 0.0149 (6) | 0.0016 (5) | 0.0032 (5) | 0.0002 (5) |
| C10 | 0.0190 (7) | 0.0197 (7) | 0.0171 (7) | 0.0024 (6) | 0.0005 (5) | −0.0015 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1—C5 | 1.3606 (17) | C4—C8 | 1.4020 (19) |
| O1—C1 | 1.3427 (17) | C5—C6 | 1.393 (2) |
| O1—C9 | 1.3835 (17) | C6—C7 | 1.377 (2) |
| O2—C3 | 1.2282 (17) | C7—C9 | 1.3946 (19) |
| O3—C10 | 1.2155 (17) | C8—C9 | 1.394 (2) |
| C1—C2 | 1.352 (2) | C1—H1 | 0.950 |
| C2—C3 | 1.4579 (19) | C4—H2 | 0.950 |
| C2—C10 | 1.4796 (18) | C6—H3 | 0.950 |
| C3—C8 | 1.4780 (18) | C7—H4 | 0.950 |
| C4—C5 | 1.3723 (18) | C10—H5 | 0.950 |
| | | | |
| O1···C3 | 2.8691 (18) | C4···H3 | 3.2823 |
| O2···C1 | 3.576 (2) | C5···H4 | 3.2513 |
| O2···C4 | 2.8658 (17) | C6···H2 | 3.2881 |
| O2···C10 | 2.8760 (18) | C8···H4 | 3.2937 |
| O3···C1 | 2.8344 (19) | C9···H1 | 3.1941 |
| C1···C7 | 3.587 (3) | C9···H2 | 3.2746 |
| C1···C8 | 2.760 (2) | C9···H3 | 3.2509 |
| C2···C9 | 2.7704 (19) | C10···H1 | 2.5600 |
| C4···C7 | 2.813 (2) | H1···H5 | 3.4953 |
| C5···C9 | 2.721 (2) | H3···H4 | 2.3436 |
| C6···C8 | 2.796 (2) | F1···H3$^{i}$ | 2.6307 |
| F1···F1$^{i}$ | 3.5513 (16) | F1···H4$^{vi}$ | 3.1761 |
| F1···F1$^{ii}$ | 3.5513 (16) | F1···H5$^{iv}$ | 3.4684 |
| F1···O2$^{iii}$ | 3.5044 (15) | F1···H5$^{v}$ | 2.6941 |
| F1···O3$^{iv}$ | 3.4981 (16) | O1···H2$^{vii}$ | 3.1318 |
| F1···O3$^{v}$ | 3.5584 (16) | O1···H4$^{xiv}$ | 2.8987 |
| F1···C6$^{i}$ | 3.315 (2) | O2···H1$^{vi}$ | 2.8570 |

| | | | |
|---|---|---|---|
| F1···C7$^{vi}$ | 3.5947 (19) | O2···H2$^{iii}$ | 2.3533 |
| F1···C10$^{iv}$ | 3.3360 (18) | O3···H1$^{x}$ | 2.3664 |
| F1···C10$^{v}$ | 3.3800 (18) | O3···H3$^{xii}$ | 2.4781 |
| O1···O2$^{vii}$ | 3.1431 (15) | O3···H4$^{xii}$ | 2.9229 |
| O1···C3$^{vii}$ | 3.5781 (19) | O3···H5$^{xi}$ | 2.9244 |
| O1···C4$^{vii}$ | 3.5315 (19) | C1···H2$^{iv}$ | 3.4844 |
| O1···C6$^{viii}$ | 3.5869 (19) | C1···H3$^{viii}$ | 3.4931 |
| O1···C7$^{viii}$ | 3.5649 (19) | C1···H4$^{xiv}$ | 3.3095 |
| O2···F1$^{iii}$ | 3.5044 (15) | C1···H5$^{xi}$ | 3.5228 |
| O2···O1$^{vi}$ | 3.1431 (15) | C2···H2$^{iv}$ | 3.4665 |
| O2···C1$^{vi}$ | 3.0162 (19) | C2···H3$^{viii}$ | 3.5928 |
| O2···C4$^{iii}$ | 3.2351 (19) | C3···H1$^{vi}$ | 3.4163 |
| O2···C7$^{iv}$ | 3.5572 (19) | C3···H2$^{iii}$ | 3.4741 |
| O2···C9$^{iv}$ | 3.4951 (19) | C3···H4$^{viii}$ | 3.4389 |
| O3···F1$^{iv}$ | 3.4981 (16) | C4···H4$^{vi}$ | 3.1477 |
| O3···F1$^{ix}$ | 3.5584 (16) | C5···H4$^{vi}$ | 3.2399 |
| O3···O3$^{x}$ | 3.3650 (17) | C5···H5$^{iv}$ | 3.4912 |
| O3···O3$^{xi}$ | 3.3650 (17) | C5···H5$^{v}$ | 3.4391 |
| O3···C1$^{x}$ | 3.3077 (19) | C6···H1$^{viii}$ | 3.5277 |
| O3···C2$^{xi}$ | 3.4099 (18) | C6···H5$^{v}$ | 3.5118 |
| O3···C6$^{xii}$ | 3.1985 (18) | C7···H2$^{vii}$ | 3.1377 |
| O3···C7$^{xii}$ | 3.4120 (19) | C8···H4$^{viii}$ | 3.5193 |
| O3···C10$^{xi}$ | 2.9773 (19) | C9···H2$^{vii}$ | 3.2243 |
| C1···O2$^{vii}$ | 3.0162 (19) | C10···H1$^{x}$ | 2.8205 |
| C1···O3$^{xi}$ | 3.3077 (19) | C10···H3$^{xii}$ | 3.2620 |
| C1···C6$^{viii}$ | 3.390 (2) | H1···O2$^{vii}$ | 2.8570 |
| C2···O3$^{x}$ | 3.4099 (18) | H1···O3$^{xi}$ | 2.3664 |
| C2···C4$^{iv}$ | 3.453 (2) | H1···C3$^{vii}$ | 3.4163 |
| C2···C5$^{iv}$ | 3.546 (2) | H1···C6$^{viii}$ | 3.5277 |
| C3···O1$^{vi}$ | 3.5781 (19) | H1···C10$^{xi}$ | 2.8205 |
| C3···C4$^{iv}$ | 3.403 (2) | H1···H3$^{viii}$ | 3.5122 |
| C3···C8$^{iv}$ | 3.461 (2) | H1···H4$^{xiv}$ | 2.9261 |
| C4···O1$^{vi}$ | 3.5315 (19) | H1···H5$^{xi}$ | 2.7690 |
| C4···O2$^{iii}$ | 3.2351 (19) | H2···O1$^{vi}$ | 3.1318 |
| C4···C2$^{iv}$ | 3.453 (2) | H2···O2$^{iii}$ | 2.3533 |
| C4···C3$^{iv}$ | 3.403 (2) | H2···C1$^{iv}$ | 3.4844 |
| C4···C7$^{vi}$ | 3.557 (3) | H2···C2$^{iv}$ | 3.4665 |
| C5···C2$^{iv}$ | 3.546 (2) | H2···C3$^{iii}$ | 3.4741 |
| C5···C10$^{iv}$ | 3.517 (2) | H2···C7$^{vi}$ | 3.1377 |
| C6···F1$^{ii}$ | 3.315 (2) | H2···C9$^{vi}$ | 3.2243 |
| C6···O1$^{viii}$ | 3.5869 (19) | H2···H2$^{iii}$ | 3.0288 |
| C6···O3$^{xiii}$ | 3.1985 (18) | H2···H4$^{vi}$ | 2.9843 |
| C6···C1$^{viii}$ | 3.390 (2) | H3···F1$^{ii}$ | 2.6307 |
| C7···F1$^{vii}$ | 3.5947 (19) | H3···O3$^{xiii}$ | 2.4781 |
| C7···O1$^{viii}$ | 3.5649 (19) | H3···C1$^{viii}$ | 3.4931 |
| C7···O2$^{iv}$ | 3.5572 (19) | H3···C2$^{viii}$ | 3.5928 |
| C7···O3$^{xiii}$ | 3.4120 (19) | H3···C10$^{xiii}$ | 3.2620 |
| C7···C4$^{vii}$ | 3.557 (3) | H3···H1$^{viii}$ | 3.5122 |

| | | | |
|---|---|---|---|
| C7···C9$^{viii}$ | 3.562 (2) | H3···H5$^{v}$ | 3.0440 |
| C8···C3$^{iv}$ | 3.461 (2) | H4···F1$^{vii}$ | 3.1761 |
| C8···C8$^{iv}$ | 3.518 (2) | H4···O1$^{xiv}$ | 2.8987 |
| C9···O2$^{iv}$ | 3.4951 (19) | H4···O3$^{xiii}$ | 2.9229 |
| C9···C7$^{viii}$ | 3.562 (2) | H4···C1$^{xiv}$ | 3.3095 |
| C9···C9$^{viii}$ | 3.374 (2) | H4···C3$^{viii}$ | 3.4389 |
| C10···F1$^{iv}$ | 3.3360 (18) | H4···C4$^{vii}$ | 3.1477 |
| C10···F1$^{ix}$ | 3.3800 (18) | H4···C5$^{vii}$ | 3.2399 |
| C10···O3$^{x}$ | 2.9773 (19) | H4···C8$^{viii}$ | 3.5193 |
| C10···C5$^{iv}$ | 3.517 (2) | H4···H1$^{xiv}$ | 2.9261 |
| F1···H2 | 2.5447 | H4···H2$^{vii}$ | 2.9843 |
| F1···H3 | 2.5415 | H5···F1$^{iv}$ | 3.4684 |
| O1···H4 | 2.5219 | H5···F1$^{ix}$ | 2.6941 |
| O2···H2 | 2.6151 | H5···O3$^{x}$ | 2.9244 |
| O2···H5 | 2.5814 | H5···C1$^{x}$ | 3.5228 |
| O3···H1 | 2.5100 | H5···C5$^{iv}$ | 3.4912 |
| C1···H5 | 3.2808 | H5···C5$^{ix}$ | 3.4391 |
| C3···H1 | 3.2935 | H5···C6$^{ix}$ | 3.5118 |
| C3···H2 | 2.6889 | H5···H1$^{x}$ | 2.7690 |
| C3···H5 | 2.6767 | H5···H3$^{ix}$ | 3.0440 |

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|---|---|---|---|
| C1—O1—C9 | 118.43 (11) | C4—C8—C9 | 118.99 (12) |
| O1—C1—C2 | 124.57 (13) | O1—C9—C7 | 116.03 (12) |
| C1—C2—C3 | 121.05 (12) | O1—C9—C8 | 121.94 (11) |
| C1—C2—C10 | 119.43 (13) | C7—C9—C8 | 122.02 (13) |
| C3—C2—C10 | 119.53 (12) | O3—C10—C2 | 124.30 (13) |
| O2—C3—C2 | 123.45 (12) | O1—C1—H1 | 117.713 |
| O2—C3—C8 | 122.66 (12) | C2—C1—H1 | 117.717 |
| C2—C3—C8 | 113.89 (12) | C5—C4—H2 | 121.008 |
| C5—C4—C8 | 117.98 (13) | C8—C4—H2 | 121.007 |
| F1—C5—C4 | 118.76 (13) | C5—C6—H3 | 120.543 |
| F1—C5—C6 | 117.91 (12) | C7—C6—H3 | 120.538 |
| C4—C5—C6 | 123.32 (13) | C6—C7—H4 | 120.618 |
| C5—C6—C7 | 118.92 (13) | C9—C7—H4 | 120.626 |
| C6—C7—C9 | 118.76 (13) | O3—C10—H5 | 117.845 |
| C3—C8—C4 | 120.90 (12) | C2—C10—H5 | 117.850 |
| C3—C8—C9 | 120.11 (12) | | |

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|---|---|---|---|
| C1—O1—C9—C7 | −179.22 (10) | C8—C4—C5—F1 | 179.77 (11) |
| C1—O1—C9—C8 | 0.80 (17) | C8—C4—C5—C6 | −0.1 (2) |
| C9—O1—C1—C2 | −1.26 (19) | H2—C4—C5—F1 | −0.2 |
| C9—O1—C1—H1 | 178.7 | H2—C4—C5—C6 | 179.9 |
| O1—C1—C2—C3 | 0.9 (2) | H2—C4—C8—C3 | 0.3 |
| O1—C1—C2—C10 | −179.01 (11) | H2—C4—C8—C9 | −179.9 |
| H1—C1—C2—C3 | −179.1 | F1—C5—C6—C7 | −179.98 (11) |
| H1—C1—C2—C10 | 1.0 | F1—C5—C6—H3 | 0.0 |
| C1—C2—C3—O2 | 179.92 (12) | C4—C5—C6—C7 | −0.1 (2) |
| C1—C2—C3—C8 | 0.01 (18) | C4—C5—C6—H3 | 179.9 |

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|---|---|---|---|
| C1—C2—C10—O3 | 2.2 (2) | C5—C6—C7—C9 | 0.4 (2) |
| C1—C2—C10—H5 | −177.8 | C5—C6—C7—H4 | −179.6 |
| C3—C2—C10—O3 | −177.66 (12) | H3—C6—C7—C9 | −179.6 |
| C3—C2—C10—H5 | 2.3 | H3—C6—C7—H4 | 0.4 |
| C10—C2—C3—O2 | −0.21 (19) | C6—C7—C9—O1 | 179.57 (11) |
| C10—C2—C3—C8 | 179.87 (11) | C6—C7—C9—C8 | −0.5 (2) |
| O2—C3—C8—C4 | −0.5 (2) | H4—C7—C9—O1 | −0.4 |
| O2—C3—C8—C9 | 179.68 (12) | H4—C7—C9—C8 | 179.6 |
| C2—C3—C8—C4 | 179.39 (11) | C3—C8—C9—O1 | 0.01 (19) |
| C2—C3—C8—C9 | −0.40 (17) | C3—C8—C9—C7 | −179.97 (11) |
| C5—C4—C8—C3 | −179.74 (11) | C4—C8—C9—O1 | −179.78 (11) |
| C5—C4—C8—C9 | 0.05 (19) | C4—C8—C9—C7 | 0.24 (19) |

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iii) −*x*, −*y*−1, −*z*+1; (iv) −*x*, −*y*, −*z*+1; (v) *x*+1/2, −*y*−1/2, *z*+1/2; (vi) *x*, *y*−1, *z*; (vii) *x*, *y*+1, *z*; (viii) −*x*+1, −*y*, −*z*+1; (ix) *x*−1/2, −*y*−1/2, *z*−1/2; (x) −*x*+1/2, *y*−1/2, −*z*+1/2; (xi) −*x*+1/2, *y*+1/2, −*z*+1/2; (xii) *x*−1/2, −*y*+1/2, *z*−1/2; (xiii) *x*+1/2, −*y*+1/2, *z*+1/2; (xiv) −*x*+1, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O3$^{xi}$ | 0.95 | 2.37 | 3.308 (2) | 171 |
| C4—H2···O2$^{iii}$ | 0.95 | 2.35 | 3.235 (2) | 154 |
| C6—H3···O3$^{xiii}$ | 0.95 | 2.48 | 3.198 (2) | 133 |

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