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2-(2-Fluorophenyl)-3-hydroxy-4*H*-chromen-4-one

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Keywords: crystal structure; flavonol; O—H···O hydrogen bonds; inversion dimer.

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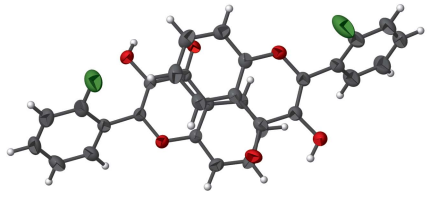
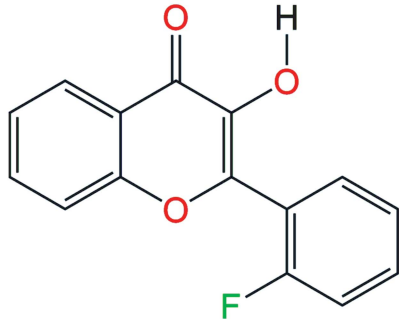
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{15}H_9FO_3$, contains two independent molecules in which the fluorine-substituted benzene ring is twisted by 47.64 (3) and 56.02 (4)° relative to the 4*H*-chromenon skeleton. The hydroxyl group in each molecule is tilted from 4*H*-chromenon skeleton by 24.5 (1) and 16.1 (1)°, respectively. In the crystal, pairs of O—H···O hydrogen bonds form inversion dimers with an $R_2^2(10)$ graph-set motif.

3D view



Chemical scheme



Structure description

Flavonoids, which include flavones, flavanone, flavonols and isoflavones, are one of the secondary metabolites in plants. Among the flavonoids, flavonols have an unique structure that has a hydroxyl group at the 3-position of the flavone backbone as an enol type. As a result of this characteristic structure, these molecules show a broad spectrum of biological activities (Patel *et al.*, 2018; Raffa *et al.*, 2017) and have applications as fluorescent probes for sensing and imaging (Serdiuk *et al.*, 2016). As a part of our studies on flavonoid derivatives (Lee *et al.*, 2014), the title compound was synthesized and its crystal structure was determined.

The title compound has two independent molecules the asymmetric unit (Fig. 1) in which the fluorine-substituted benzene rings are connected at the C8 and C23 positions of the 4*H*-chromenon skeleton. The dihedral angles between these rings and the 4*H*-chromenon skeleton are 47.64 (3) and 56.02 (4)°, respectively. As a consequence of the flavonol structure, the hydroxyl groups are attached at the C9 and C24 positions of the 4*H*-chromenon skeletons and are tilted from 4*H*-chromenon ring system by 24.5 (1)° (C1/C9/O3/H3*A*) and 16.1 (1)° (C61/C24/O6/H6*A*).

In the crystal, pairs of intermolecular O—H···O hydrogen bonds form inversion dimers with $R_2^2(10)$ graph-set motifs (Table 1, Fig. 2).

Examples of other flavonol structures have also been published recently, see Padgett *et al.* (2018) and Narita *et al.* (2015).

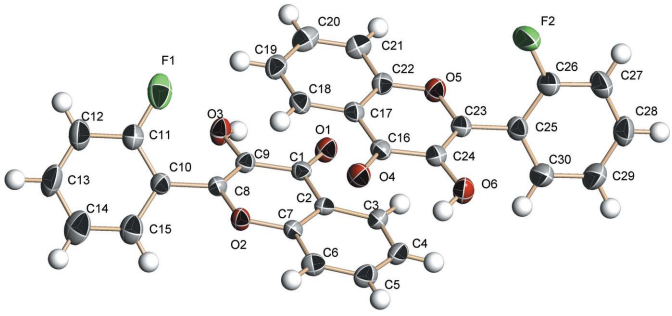


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level.

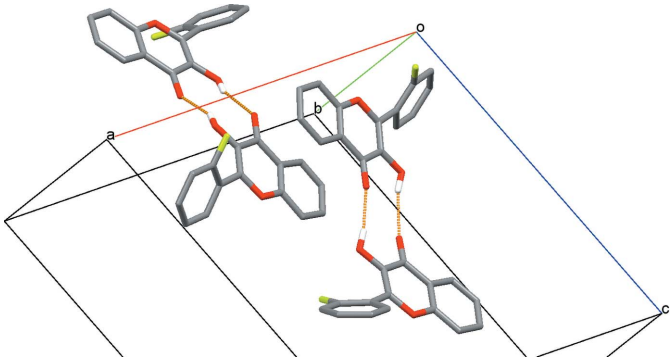


Figure 2
Part of the crystal structure with intermolecular hydrogen bonds are shown as dashed lines. For clarity only those H atoms involved in hydrogen bonding are shown.

Synthesis and crystallization

The starting material, chalcone **I**, was prepared by previously reported methods (Yoo *et al.*, 2014). The final flavonol product was obtained by oxidative cyclization of the **I** with H_2O_2 in an alkaline methanol medium (Fig. 3).

Refinement

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

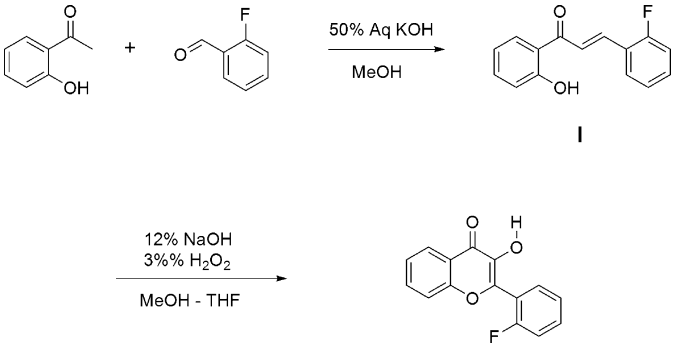


Figure 3
Synthetic scheme for the preparation of the title compound.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O4^{i}	0.83	1.91	2.6813 (18)	154
O6—H6A···O1^{ii}	0.83	2.04	2.8112 (18)	154

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_9FO_3$
M_r	256.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	223
a, b, c (Å)	22.3701 (6), 6.8836 (2), 15.7987 (4)
β (°)	106.0575 (13)
V (Å^3)	2337.87 (11)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.19 × 0.14 × 0.10
Data collection	
Diffractometer	Bruker PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker 2012)
T_{min}, T_{max}	0.979, 0.989
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	68936, 5842, 3646
R_{int}	0.086
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.134, 1.03
No. of reflections	5842
No. of parameters	345
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.30

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

Funding information

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References

Bruker (2012). *APEX2*, *SAINT* and *SADABS*, Bruker AXS Inc. Madison, Wisconsin, USA.
Lee, M. S., Yong, Y., Lee, J. M., Koh, D., Shin, S. Y. & Lee, Y. H. (2014). *J. Korean Soc. Appl. Biol. Chem.* **57**, 129–132.
Narita, F., Takura, A. & Fujihara, T. (2015). *Acta Cryst.* E**71**, 824–826.
Padgett, C. W., Lynch, W. L., Sheriff, K., Dean, R. & Zingales, S. (2018). *IUCrData*, **3**, x181138.
Patel, R. V., Mistry, B. M., Shinde, S. K., Syed, R., Singh, V. & Shin, H. S. (2018). *Eur. J. Med. Chem.* **155**, 889–904.
Raffa, D., Maggio, B., Raimondi, M. V., Plescia, F. & Daidone, G. (2017). *Eur. J. Med. Chem.* **142**, 213–228.
Serdiuk, I. E., Reszka, M., Myszka, H., Krzymiński, K., Liberek, B. & Roshal, A. D. (2016). *RSC Adv.* **6**, 42532–42536.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yoo, J. S., Lim, Y. & Koh, D. (2014). *Acta Cryst.* E**70**, o999–o1000.

full crystallographic data

IUCrData (2018). **3**, x181332 [https://doi.org/10.1107/S2414314618013329]

2-(2-Fluorophenyl)-3-hydroxy-4*H*-chromen-4-one

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2-(2-Fluorophenyl)-3-hydroxy-4*H*-chromen-4-one

Crystal data

$C_{15}H_9FO_3$
M_r = 256.22
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 22.3701 (6) Å
b = 6.8836 (2) Å
c = 15.7987 (4) Å
β = 106.0575 (13)°
V = 2337.87 (11) Å^3
Z = 8
$F(000)$ = 1056
D_x = 1.456 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9839 reflections
θ = 2.6–27.2°
μ = 0.11 mm^{-1}
T = 223 K
Block, yellow
0.19 × 0.14 × 0.10 mm

Data collection

Bruker PHOTON 100 CMOS diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker 2012)
T_{min} = 0.979, T_{max} = 0.989
68936 measured reflections
5842 independent reflections
3646 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 28.4°, θ_{min} = 2.6°
h = −29→29
k = −9→9
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.134
S = 1.03
5842 reflections
345 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
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.8816P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 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}
C1	0.25573 (8)	0.8644 (2)	0.03626 (11)	0.0274 (4)
O1	0.21337 (5)	0.85797 (19)	−0.03333 (8)	0.0372 (3)
C2	0.24556 (7)	0.8811 (2)	0.12298 (10)	0.0261 (3)
C3	0.18533 (8)	0.8880 (2)	0.13403 (12)	0.0324 (4)
H3	0.1504	0.8791	0.0847	0.039*
C4	0.17746 (9)	0.9077 (3)	0.21655 (12)	0.0372 (4)
H4	0.1371	0.9133	0.2237	0.045*
C5	0.22892 (9)	0.9196 (3)	0.28987 (13)	0.0400 (5)
H5	0.2230	0.9312	0.3463	0.048*
C6	0.28829 (9)	0.9144 (3)	0.28110 (12)	0.0367 (4)
H6	0.3230	0.9240	0.3307	0.044*
C7	0.29576 (8)	0.8948 (2)	0.19709 (11)	0.0286 (4)
O2	0.35602 (5)	0.88921 (18)	0.19202 (7)	0.0321 (3)
C8	0.36710 (8)	0.8753 (2)	0.11136 (11)	0.0279 (4)
C9	0.32064 (8)	0.8628 (2)	0.03648 (11)	0.0287 (4)
O3	0.33412 (6)	0.8547 (2)	−0.04188 (8)	0.0413 (3)
H3A	0.3045	0.8987	−0.0811	0.062*
C10	0.43386 (8)	0.8899 (3)	0.11802 (11)	0.0324 (4)
C11	0.46360 (9)	0.7656 (3)	0.07444 (13)	0.0412 (5)
F1	0.43134 (6)	0.61549 (18)	0.02827 (10)	0.0632 (4)
C12	0.52522 (9)	0.7845 (4)	0.07719 (15)	0.0533 (6)
H12	0.5438	0.6974	0.0462	0.064*
C13	0.55925 (10)	0.9320 (4)	0.12567 (15)	0.0577 (6)
H13	0.6013	0.9481	0.1274	0.069*
C14	0.53195 (10)	1.0561 (4)	0.17168 (15)	0.0596 (6)
H14	0.5556	1.1561	0.2056	0.072*
C15	0.46989 (9)	1.0353 (3)	0.16852 (13)	0.0462 (5)
H15	0.4518	1.1205	0.2009	0.055*
C16	0.22946 (8)	0.4205 (2)	0.24636 (11)	0.0308 (4)
O4	0.26839 (6)	0.4421 (2)	0.31850 (8)	0.0430 (3)
C17	0.24559 (8)	0.3890 (2)	0.16460 (11)	0.0291 (4)
C18	0.30774 (8)	0.3875 (3)	0.16103 (13)	0.0362 (4)
H18	0.3402	0.4067	0.2128	0.043*
C19	0.32119 (9)	0.3584 (3)	0.08274 (13)	0.0409 (5)
H19	0.3628	0.3583	0.0807	0.049*
C20	0.27342 (10)	0.3288 (3)	0.00602 (13)	0.0431 (5)
H20	0.2832	0.3087	−0.0475	0.052*
C21	0.21241 (9)	0.3284 (3)	0.00727 (12)	0.0387 (4)
H21	0.1803	0.3077	−0.0447	0.046*
C22	0.19908 (8)	0.3595 (2)	0.08723 (11)	0.0311 (4)

O5	0.13760 (5)	0.35843 (18)	0.08520 (8)	0.0358 (3)
C23	0.12074 (8)	0.3917 (2)	0.16077 (11)	0.0312 (4)
C24	0.16363 (8)	0.4237 (2)	0.23858 (11)	0.0316 (4)
O6	0.14504 (6)	0.4531 (2)	0.31246 (8)	0.0426 (3)
H6A	0.1745	0.4970	0.3520	0.064*
C25	0.05281 (8)	0.3874 (3)	0.14600 (12)	0.0355 (4)
C26	0.01747 (9)	0.2293 (3)	0.10776 (13)	0.0422 (5)
F2	0.04694 (6)	0.07393 (19)	0.08650 (10)	0.0716 (4)
C27	−0.04596 (9)	0.2209 (3)	0.09268 (14)	0.0482 (5)
H27	−0.0684	0.1103	0.0669	0.058*
C28	−0.07580 (9)	0.3772 (3)	0.11595 (14)	0.0487 (5)
H28	−0.1193	0.3750	0.1053	0.058*
C29	−0.04274 (10)	0.5372 (4)	0.15475 (15)	0.0554 (6)
H29	−0.0636	0.6435	0.1708	0.066*
C30	0.02118 (9)	0.5420 (3)	0.17027 (15)	0.0490 (5)
H30	0.0435	0.6514	0.1976	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0271 (9)	0.0263 (8)	0.0275 (9)	−0.0021 (7)	0.0054 (7)	0.0013 (7)
O1	0.0287 (7)	0.0501 (8)	0.0295 (6)	−0.0063 (6)	0.0026 (5)	−0.0006 (6)
C2	0.0282 (9)	0.0226 (8)	0.0279 (8)	0.0011 (7)	0.0081 (7)	0.0030 (7)
C3	0.0290 (9)	0.0318 (9)	0.0376 (10)	−0.0017 (7)	0.0112 (8)	0.0039 (8)
C4	0.0362 (10)	0.0375 (10)	0.0439 (11)	0.0002 (8)	0.0209 (9)	0.0039 (8)
C5	0.0479 (12)	0.0434 (11)	0.0352 (10)	0.0020 (9)	0.0225 (9)	0.0018 (8)
C6	0.0399 (11)	0.0428 (11)	0.0271 (9)	0.0015 (8)	0.0088 (8)	0.0021 (8)
C7	0.0278 (9)	0.0286 (8)	0.0297 (9)	0.0033 (7)	0.0089 (7)	0.0041 (7)
O2	0.0262 (6)	0.0441 (7)	0.0254 (6)	0.0037 (5)	0.0063 (5)	0.0031 (5)
C8	0.0264 (9)	0.0297 (9)	0.0280 (9)	0.0026 (7)	0.0084 (7)	0.0026 (7)
C9	0.0296 (9)	0.0313 (9)	0.0266 (8)	−0.0002 (7)	0.0102 (7)	−0.0001 (7)
O3	0.0305 (7)	0.0674 (9)	0.0271 (6)	0.0021 (6)	0.0097 (5)	0.0011 (6)
C10	0.0260 (9)	0.0413 (10)	0.0283 (9)	0.0006 (7)	0.0050 (7)	0.0053 (8)
C11	0.0325 (10)	0.0454 (11)	0.0465 (11)	0.0006 (9)	0.0124 (9)	0.0012 (9)
F1	0.0482 (8)	0.0545 (8)	0.0928 (10)	−0.0020 (6)	0.0290 (7)	−0.0240 (7)
C12	0.0358 (11)	0.0753 (16)	0.0522 (13)	0.0082 (11)	0.0182 (10)	0.0014 (12)
C13	0.0268 (10)	0.0963 (19)	0.0498 (13)	−0.0072 (12)	0.0106 (10)	0.0082 (13)
C14	0.0369 (12)	0.0849 (18)	0.0508 (13)	−0.0174 (12)	0.0019 (10)	−0.0093 (12)
C15	0.0332 (11)	0.0613 (13)	0.0406 (11)	−0.0052 (10)	0.0046 (9)	−0.0061 (10)
C16	0.0287 (9)	0.0280 (9)	0.0338 (10)	−0.0002 (7)	0.0054 (8)	−0.0011 (7)
O4	0.0313 (7)	0.0576 (9)	0.0349 (7)	0.0013 (6)	0.0003 (6)	−0.0104 (6)
C17	0.0291 (9)	0.0230 (8)	0.0349 (9)	−0.0001 (7)	0.0080 (7)	0.0013 (7)
C18	0.0322 (10)	0.0305 (9)	0.0455 (11)	−0.0020 (7)	0.0101 (8)	−0.0007 (8)
C19	0.0403 (11)	0.0333 (10)	0.0553 (12)	0.0005 (8)	0.0234 (10)	0.0042 (9)
C20	0.0558 (13)	0.0396 (11)	0.0404 (11)	0.0072 (9)	0.0241 (10)	0.0088 (9)
C21	0.0437 (11)	0.0399 (10)	0.0315 (10)	0.0066 (9)	0.0086 (8)	0.0044 (8)
C22	0.0304 (9)	0.0276 (9)	0.0356 (9)	0.0032 (7)	0.0095 (8)	0.0040 (7)
O5	0.0290 (7)	0.0454 (7)	0.0307 (6)	0.0025 (5)	0.0044 (5)	−0.0013 (6)

C23	0.0277 (9)	0.0319 (9)	0.0328 (9)	0.0009 (7)	0.0065 (7)	−0.0009 (7)
C24	0.0305 (9)	0.0320 (9)	0.0322 (9)	−0.0004 (7)	0.0082 (8)	−0.0005 (7)
O6	0.0311 (7)	0.0640 (9)	0.0334 (7)	−0.0041 (6)	0.0098 (6)	−0.0072 (6)
C25	0.0281 (9)	0.0420 (10)	0.0335 (10)	0.0000 (8)	0.0039 (8)	−0.0002 (8)
C26	0.0314 (10)	0.0439 (11)	0.0471 (11)	0.0032 (8)	0.0040 (9)	−0.0070 (9)
F2	0.0407 (7)	0.0566 (8)	0.1086 (12)	0.0017 (6)	0.0058 (7)	−0.0330 (8)
C27	0.0313 (11)	0.0542 (13)	0.0532 (13)	−0.0062 (9)	0.0019 (9)	−0.0053 (10)
C28	0.0266 (10)	0.0677 (14)	0.0494 (12)	0.0016 (10)	0.0066 (9)	0.0003 (11)
C29	0.0359 (12)	0.0623 (15)	0.0674 (15)	0.0088 (10)	0.0135 (11)	−0.0127 (12)
C30	0.0370 (11)	0.0481 (12)	0.0599 (13)	0.0022 (9)	0.0098 (10)	−0.0133 (10)

Geometric parameters (Å, º)

C1—O1	1.238 (2)	C16—O4	1.237 (2)
C1—C9	1.451 (2)	C16—C24	1.444 (2)
C1—C2	1.454 (2)	C16—C17	1.450 (2)
C2—C7	1.383 (2)	C17—C22	1.384 (2)
C2—C3	1.406 (2)	C17—C18	1.407 (2)
C3—C4	1.370 (2)	C18—C19	1.366 (3)
C3—H3	0.9400	C18—H18	0.9400
C4—C5	1.391 (3)	C19—C20	1.391 (3)
C4—H4	0.9400	C19—H19	0.9400
C5—C6	1.373 (3)	C20—C21	1.370 (3)
C5—H5	0.9400	C20—H20	0.9400
C6—C7	1.389 (2)	C21—C22	1.392 (2)
C6—H6	0.9400	C21—H21	0.9400
C7—O2	1.3728 (19)	C22—O5	1.367 (2)
O2—C8	1.3671 (19)	O5—C23	1.367 (2)
C8—C9	1.344 (2)	C23—C24	1.352 (2)
C8—C10	1.471 (2)	C23—C25	1.473 (2)
C9—O3	1.3539 (19)	C24—O6	1.358 (2)
O3—H3A	0.8300	O6—H6A	0.8300
C10—C11	1.379 (3)	C25—C26	1.382 (3)
C10—C15	1.390 (3)	C25—C30	1.390 (3)
C11—F1	1.353 (2)	C26—F2	1.346 (2)
C11—C12	1.373 (3)	C26—C27	1.374 (3)
C12—C13	1.369 (3)	C27—C28	1.369 (3)
C12—H12	0.9400	C27—H27	0.9400
C13—C14	1.370 (3)	C28—C29	1.373 (3)
C13—H13	0.9400	C28—H28	0.9400
C14—C15	1.383 (3)	C29—C30	1.383 (3)
C14—H14	0.9400	C29—H29	0.9400
C15—H15	0.9400	C30—H30	0.9400
O1—C1—C9	121.44 (15)	O4—C16—C24	121.22 (16)
O1—C1—C2	123.96 (15)	O4—C16—C17	123.60 (16)
C9—C1—C2	114.56 (14)	C24—C16—C17	115.19 (15)
C7—C2—C3	118.29 (15)	C22—C17—C18	118.26 (16)

C7—C2—C1	120.05 (14)	C22—C17—C16	119.82 (15)
C3—C2—C1	121.64 (15)	C18—C17—C16	121.92 (16)
C4—C3—C2	120.08 (17)	C19—C18—C17	120.32 (18)
C4—C3—H3	120.0	C19—C18—H18	119.8
C2—C3—H3	120.0	C17—C18—H18	119.8
C3—C4—C5	120.24 (17)	C18—C19—C20	120.12 (18)
C3—C4—H4	119.9	C18—C19—H19	119.9
C5—C4—H4	119.9	C20—C19—H19	119.9
C6—C5—C4	121.00 (17)	C21—C20—C19	121.04 (18)
C6—C5—H5	119.5	C21—C20—H20	119.5
C4—C5—H5	119.5	C19—C20—H20	119.5
C5—C6—C7	118.29 (17)	C20—C21—C22	118.48 (18)
C5—C6—H6	120.9	C20—C21—H21	120.8
C7—C6—H6	120.9	C22—C21—H21	120.8
O2—C7—C2	121.94 (14)	O5—C22—C17	121.83 (15)
O2—C7—C6	115.97 (15)	O5—C22—C21	116.39 (16)
C2—C7—C6	122.08 (15)	C17—C22—C21	121.78 (16)
C8—O2—C7	119.38 (13)	C22—O5—C23	119.83 (13)
C9—C8—O2	121.96 (14)	C24—C23—O5	121.57 (15)
C9—C8—C10	126.14 (15)	C24—C23—C25	126.09 (16)
O2—C8—C10	111.76 (14)	O5—C23—C25	112.33 (14)
C8—C9—O3	119.60 (15)	C23—C24—O6	119.78 (15)
C8—C9—C1	122.08 (15)	C23—C24—C16	121.71 (16)
O3—C9—C1	118.28 (14)	O6—C24—C16	118.47 (15)
C9—O3—H3A	109.5	C24—O6—H6A	109.5
C11—C10—C15	116.74 (17)	C26—C25—C30	116.78 (17)
C11—C10—C8	122.85 (17)	C26—C25—C23	121.72 (16)
C15—C10—C8	120.40 (16)	C30—C25—C23	121.50 (17)
F1—C11—C12	118.08 (18)	F2—C26—C27	118.48 (18)
F1—C11—C10	118.95 (16)	F2—C26—C25	118.31 (16)
C12—C11—C10	123.0 (2)	C27—C26—C25	123.19 (18)
C13—C12—C11	119.1 (2)	C28—C27—C26	118.5 (2)
C13—C12—H12	120.5	C28—C27—H27	120.7
C11—C12—H12	120.5	C26—C27—H27	120.7
C12—C13—C14	119.91 (19)	C27—C28—C29	120.53 (19)
C12—C13—H13	120.0	C27—C28—H28	119.7
C14—C13—H13	120.0	C29—C28—H28	119.7
C13—C14—C15	120.4 (2)	C28—C29—C30	120.1 (2)
C13—C14—H14	119.8	C28—C29—H29	119.9
C15—C14—H14	119.8	C30—C29—H29	119.9
C14—C15—C10	120.8 (2)	C29—C30—C25	120.9 (2)
C14—C15—H15	119.6	C29—C30—H30	119.6
C10—C15—H15	119.6	C25—C30—H30	119.6

O1—C1—C2—C7	−177.53 (16)	O4—C16—C17—C22	177.76 (16)
C9—C1—C2—C7	0.3 (2)	C24—C16—C17—C22	−1.7 (2)
O1—C1—C2—C3	1.0 (3)	O4—C16—C17—C18	−2.3 (3)
C9—C1—C2—C3	178.91 (15)	C24—C16—C17—C18	178.18 (16)

C7—C2—C3—C4	−0.1 (2)	C22—C17—C18—C19	0.3 (3)
C1—C2—C3—C4	−178.66 (15)	C16—C17—C18—C19	−179.66 (16)
C2—C3—C4—C5	−0.5 (3)	C17—C18—C19—C20	−0.4 (3)
C3—C4—C5—C6	0.9 (3)	C18—C19—C20—C21	0.1 (3)
C4—C5—C6—C7	−0.8 (3)	C19—C20—C21—C22	0.3 (3)
C3—C2—C7—O2	179.99 (14)	C18—C17—C22—O5	179.88 (15)
C1—C2—C7—O2	−1.4 (2)	C16—C17—C22—O5	−0.2 (2)
C3—C2—C7—C6	0.2 (2)	C18—C17—C22—C21	0.2 (2)
C1—C2—C7—C6	178.81 (16)	C16—C17—C22—C21	−179.93 (16)
C5—C6—C7—O2	−179.60 (15)	C20—C21—C22—O5	179.81 (16)
C5—C6—C7—C2	0.2 (3)	C20—C21—C22—C17	−0.5 (3)
C2—C7—O2—C8	1.9 (2)	C17—C22—O5—C23	1.6 (2)
C6—C7—O2—C8	−178.26 (15)	C21—C22—O5—C23	−178.70 (15)
C7—O2—C8—C9	−1.4 (2)	C22—O5—C23—C24	−0.8 (2)
C7—O2—C8—C10	174.60 (14)	C22—O5—C23—C25	179.34 (14)
O2—C8—C9—O3	178.22 (15)	O5—C23—C24—O6	−178.93 (15)
C10—C8—C9—O3	2.8 (3)	C25—C23—C24—O6	0.9 (3)
O2—C8—C9—C1	0.4 (3)	O5—C23—C24—C16	−1.3 (3)
C10—C8—C9—C1	−175.02 (16)	C25—C23—C24—C16	178.54 (16)
O1—C1—C9—C8	178.06 (16)	O4—C16—C24—C23	−177.03 (17)
C2—C1—C9—C8	0.1 (2)	C17—C16—C24—C23	2.5 (2)
O1—C1—C9—O3	0.2 (3)	O4—C16—C24—O6	0.7 (3)
C2—C1—C9—O3	−177.70 (14)	C17—C16—C24—O6	−179.83 (15)
C9—C8—C10—C11	−49.9 (3)	C24—C23—C25—C26	−124.8 (2)
O2—C8—C10—C11	134.25 (17)	O5—C23—C25—C26	55.0 (2)
C9—C8—C10—C15	128.9 (2)	C24—C23—C25—C30	54.9 (3)
O2—C8—C10—C15	−46.9 (2)	O5—C23—C25—C30	−125.27 (19)
C15—C10—C11—F1	176.51 (17)	C30—C25—C26—F2	−177.54 (18)
C8—C10—C11—F1	−4.6 (3)	C23—C25—C26—F2	2.2 (3)
C15—C10—C11—C12	−2.0 (3)	C30—C25—C26—C27	0.6 (3)
C8—C10—C11—C12	176.81 (19)	C23—C25—C26—C27	−179.67 (19)
F1—C11—C12—C13	−178.09 (19)	F2—C26—C27—C28	178.68 (19)
C10—C11—C12—C13	0.5 (3)	C25—C26—C27—C28	0.5 (3)
C11—C12—C13—C14	1.1 (3)	C26—C27—C28—C29	−1.0 (3)
C12—C13—C14—C15	−0.9 (4)	C27—C28—C29—C30	0.3 (4)
C13—C14—C15—C10	−0.7 (3)	C28—C29—C30—C25	0.9 (4)
C11—C10—C15—C14	2.1 (3)	C26—C25—C30—C29	−1.3 (3)
C8—C10—C15—C14	−176.75 (19)	C23—C25—C30—C29	179.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O4^{i}	0.83	1.91	2.6813 (18)	154
O6—H6*A*···O1^{ii}	0.83	2.04	2.8112 (18)	154

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