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2-(5-Methyl-1-benzofuran-3-yl)acetic acid

N. Ramprasad,[a] Ramakrishna Gowda,[b]* K. V. Arjuna Gowda[c] and Mahantesha Basanagouda[d]

[a]Department of Physics, Govt. First Grade College, Mulbagal, Kolar dist 563 131, Karnataka, India, [b]Department of Physics, Govt. College for Women, Kolar 563 101, Karnataka, India, [c]Department of Physics, Govt. College for Women, Mandya 571 401, India, and [d]Department of Chemistry, P.C. Jabin Science College, Hubli 580 031, Karnataka, India. *Correspondence e-mail: rkgowdaphy@gmail.com

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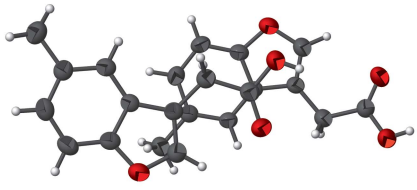
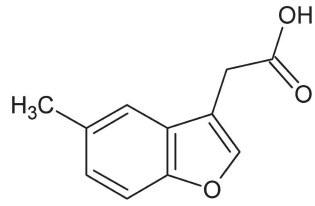
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{11}H_{10}O_3$, contains two crystallographically independent molecules, *A* and *B*, with closely matching conformations (r.m.s. overlay fit = 0.105 Å). In each case, the OH group of the acetic acid residue occupies a position approximately antiperiplanar to the C atom of the heterocycle. A short intramolecular C—H···O contact occurs within each molecule. In the crystal, carboxylic acid *A*+*B* dimers generate $R_2^2(8)$ loops.

3D view



Chemical scheme



Structure description

Derivatives of 2,3-dihydro-benzofuranyl-3-acetic acids have been reported to be potent, selective and orally bioavailable G protein-coupled receptor 40 (GPR40) and free fatty acid receptor 1 agonists (FFA1) as glucose-dependent insulinotropic agents (Negoro *et al.* 2012). As part of our studies in this area, we now report the synthesis and crystal structure of the title compound.

All the bond lengths and angles of the title molecule are close to those observed for a similar structure (Gowda *et al.*, 2015). The asymmetric unit of the title compound contains two crystallographically independent molecules (C1–C11,O1–O3 and C12–C22,O4–O6), which are almost identical (Fig. 1). In each molecule there is an intramolecular C—H···O contact present (Table 1). In the crystal, molecules are linked *via* pairs of O—H···O hydrogen bonds, forming *A*–*B* dimers (Table 1 and Fig. 2).

Synthesis and crystallization

6-Methyl-4-bromomethylcoumarin (10 m*M*) was refluxed in 1 *M* NaOH (100 ml) for 2 h (the completion of the reaction was monitored by TLC). The reaction mixture was

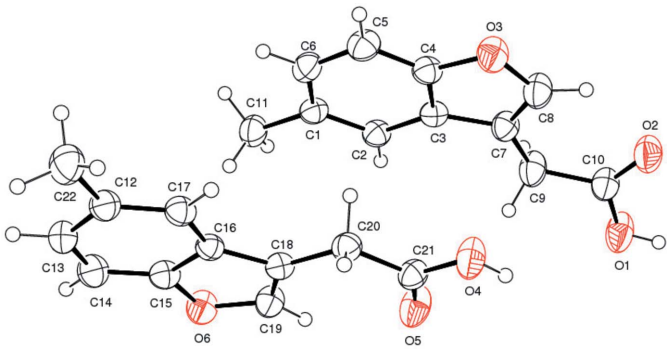


Figure 1
The molecular structure of the title compound, showing 40% probability displacement ellipsoids.

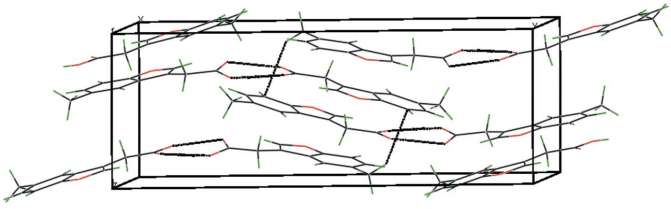


Figure 2
The crystal packing diagram of the title compound. The dotted lines indicate hydrogen bonds. All H atoms not involved in interactions have been omitted for clarity.

cooled, neutralized with 1 *M* HCl and the obtained product was filtered and dried. Colourless blocks were obtained by recrystallization from an ethanol and ethyl acetate solvent mixture by slow evaporation technique (m.p. 370–371 K) (Basanagouda *et al.* 2015).

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O5^{i}	0.82	1.83	2.650 (2)	176
O4—H4A···O2^{ii}	0.82	1.90	2.715 (2)	179
C8—H8···O2	0.93	2.29	2.855 (3)	118
C19—H19···O5	0.93	2.29	2.843 (3)	118

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_{10}O_3$
M_r	190.19
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	12.2090 (5), 20.3796 (14), 7.4335 (9)
β (°)	95.980 (4)
V (Å^3)	1839.5 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.35 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.964, 0.989
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21006, 3240, 2051
R_{int}	0.052
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.115, 1.02
No. of reflections	3240
No. of parameters	256
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.16

Computer programs: *APEX2* (Bruker, 2004), *SAINT* (Bruker, 2004), *SIR92* (Altomare *et al.*, 1994), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Bruno *et al.*, 2002).

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full crystallographic data

IUCrData (2016). **1**, x160170 [https://doi.org/10.1107/S241431461600170X]

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2-(5-Methyl-1-benzofuran-3-yl)acetic acid

Crystal data

$C_{11}H_{10}O_3$
M_r = 190.19
Monoclinic, $P2_1/c$
a = 12.2090 (5) Å
b = 20.3796 (14) Å
c = 7.4335 (9) Å
β = 95.980 (4)°
V = 1839.5 (3) Å^3
Z = 8
$F(000)$ = 800
D_x = 1.373 Mg m^{-3}
Melting point = 370–371 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4172 reflections
θ = 2.9–23.9°
μ = 0.10 mm^{-1}
T = 296 K
Block, colourless
0.35 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.964, T_{max} = 0.989
21006 measured reflections
3240 independent reflections
2051 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 25.0°, θ_{min} = 2.6°
h = −14→14
k = −24→24
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.02
3240 reflections
256 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.4188P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0026 (6)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.81759 (17)	0.05868 (10)	0.6079 (3)	0.0399 (5)
C2	0.83597 (17)	−0.00743 (10)	0.6377 (2)	0.0396 (5)
H2	0.9059	−0.0249	0.6315	0.048*
C3	0.75005 (16)	−0.04785 (10)	0.6770 (2)	0.0363 (5)
C4	0.64678 (17)	−0.02035 (11)	0.6843 (3)	0.0412 (5)
C5	0.62420 (18)	0.04512 (11)	0.6551 (3)	0.0482 (6)
H5	0.5541	0.0623	0.6604	0.058*
C6	0.71189 (18)	0.08378 (11)	0.6174 (3)	0.0467 (6)
H6	0.7001	0.1284	0.5976	0.056*
C7	0.73877 (17)	−0.11645 (10)	0.7170 (3)	0.0423 (5)
C8	0.63338 (19)	−0.12474 (11)	0.7455 (3)	0.0530 (6)
H8	0.6038	−0.1649	0.7747	0.064*
C9	0.83049 (18)	−0.16488 (10)	0.7216 (3)	0.0539 (6)
H9A	0.8660	−0.1597	0.6117	0.065*
H9B	0.8843	−0.1536	0.8222	0.065*
C10	0.8017 (2)	−0.23539 (11)	0.7389 (3)	0.0493 (6)
C11	0.90915 (18)	0.10371 (11)	0.5656 (3)	0.0508 (6)
H11A	0.9788	0.0833	0.6019	0.076*
H11B	0.9041	0.1443	0.6300	0.076*
H11C	0.9029	0.1123	0.4380	0.076*
C12	0.66060 (18)	0.20598 (11)	0.0042 (3)	0.0442 (5)
C13	0.76168 (19)	0.23023 (11)	−0.0384 (3)	0.0491 (6)
H13	0.7650	0.2730	−0.0810	0.059*
C14	0.85690 (18)	0.19330 (11)	−0.0201 (3)	0.0497 (6)
H14	0.9241	0.2103	−0.0464	0.060*
C15	0.84690 (17)	0.13011 (11)	0.0392 (3)	0.0419 (5)
C16	0.74906 (16)	0.10295 (10)	0.0811 (2)	0.0357 (5)
C17	0.65453 (17)	0.14192 (10)	0.0641 (3)	0.0416 (5)
H17	0.5878	0.1249	0.0929	0.050*
C18	0.77211 (17)	0.03530 (10)	0.1269 (3)	0.0376 (5)
C19	0.87940 (18)	0.02707 (11)	0.1095 (3)	0.0472 (6)
H19	0.9163	−0.0126	0.1301	0.057*
C20	0.68777 (17)	−0.01216 (10)	0.1778 (3)	0.0425 (5)
H20A	0.6595	0.0039	0.2867	0.051*
H20B	0.6271	−0.0120	0.0826	0.051*
C21	0.72311 (19)	−0.08114 (10)	0.2101 (3)	0.0430 (5)
C22	0.56094 (19)	0.24951 (12)	−0.0157 (3)	0.0616 (7)
H22A	0.4962	0.2233	−0.0449	0.092*
H22B	0.5677	0.2807	−0.1107	0.092*
H22C	0.5552	0.2724	0.0958	0.092*
O1	0.88003 (13)	−0.27454 (8)	0.6973 (3)	0.0706 (5)
H1A	0.8580	−0.3126	0.6958	0.085*
O2	0.71609 (14)	−0.25546 (8)	0.7889 (2)	0.0660 (5)
O3	0.57310 (12)	−0.06757 (7)	0.7271 (2)	0.0544 (4)
O4	0.64091 (12)	−0.11960 (7)	0.2445 (2)	0.0620 (5)

H4A	0.6631	−0.1575	0.2574	0.074*
O5	0.81643 (13)	−0.10129 (7)	0.2076 (2)	0.0623 (5)
O6	0.92925 (11)	0.08380 (7)	0.0578 (2)	0.0516 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0400 (13)	0.0407 (13)	0.0390 (11)	−0.0006 (10)	0.0046 (9)	−0.0054 (10)
C2	0.0330 (12)	0.0421 (13)	0.0442 (12)	0.0009 (10)	0.0059 (9)	−0.0025 (10)
C3	0.0330 (12)	0.0402 (12)	0.0355 (11)	−0.0001 (10)	0.0024 (9)	−0.0034 (9)
C4	0.0346 (13)	0.0455 (14)	0.0441 (12)	−0.0026 (11)	0.0064 (10)	−0.0047 (10)
C5	0.0376 (13)	0.0485 (15)	0.0587 (14)	0.0076 (11)	0.0061 (11)	−0.0026 (11)
C6	0.0496 (14)	0.0378 (13)	0.0531 (13)	0.0053 (11)	0.0072 (11)	−0.0012 (10)
C7	0.0357 (13)	0.0402 (13)	0.0507 (13)	−0.0037 (10)	0.0036 (10)	−0.0015 (10)
C8	0.0468 (15)	0.0422 (14)	0.0704 (16)	−0.0037 (12)	0.0085 (12)	0.0026 (12)
C9	0.0419 (14)	0.0412 (14)	0.0791 (16)	−0.0035 (11)	0.0081 (12)	0.0046 (12)
C10	0.0429 (14)	0.0405 (14)	0.0645 (15)	−0.0001 (12)	0.0060 (12)	0.0029 (11)
C11	0.0501 (14)	0.0413 (13)	0.0622 (14)	−0.0046 (11)	0.0113 (11)	0.0004 (11)
C12	0.0468 (14)	0.0434 (13)	0.0422 (12)	0.0026 (11)	0.0040 (10)	0.0003 (10)
C13	0.0588 (16)	0.0400 (13)	0.0493 (13)	−0.0039 (12)	0.0096 (11)	0.0025 (10)
C14	0.0431 (14)	0.0505 (15)	0.0564 (14)	−0.0101 (12)	0.0099 (11)	−0.0013 (11)
C15	0.0365 (13)	0.0466 (14)	0.0429 (12)	−0.0016 (11)	0.0048 (10)	−0.0043 (10)
C16	0.0358 (12)	0.0389 (12)	0.0324 (11)	−0.0026 (10)	0.0032 (9)	−0.0027 (9)
C17	0.0374 (13)	0.0454 (13)	0.0425 (12)	−0.0015 (10)	0.0070 (10)	−0.0011 (10)
C18	0.0360 (13)	0.0394 (13)	0.0375 (11)	0.0003 (10)	0.0039 (9)	−0.0033 (9)
C19	0.0458 (15)	0.0405 (14)	0.0552 (14)	0.0004 (11)	0.0056 (11)	0.0002 (11)
C20	0.0422 (13)	0.0413 (13)	0.0442 (12)	0.0015 (10)	0.0060 (10)	−0.0015 (10)
C21	0.0407 (14)	0.0402 (13)	0.0478 (13)	−0.0034 (12)	0.0029 (10)	−0.0051 (10)
C22	0.0600 (16)	0.0539 (15)	0.0712 (17)	0.0101 (13)	0.0086 (13)	0.0099 (13)
O1	0.0501 (10)	0.0396 (10)	0.1260 (15)	0.0026 (8)	0.0271 (10)	0.0054 (9)
O2	0.0561 (11)	0.0432 (10)	0.1032 (14)	−0.0048 (9)	0.0294 (10)	0.0024 (9)
O3	0.0375 (9)	0.0498 (10)	0.0772 (11)	−0.0027 (8)	0.0120 (8)	0.0010 (8)
O4	0.0472 (10)	0.0385 (9)	0.1025 (13)	−0.0004 (8)	0.0182 (9)	0.0061 (9)
O5	0.0395 (10)	0.0424 (10)	0.1051 (13)	0.0036 (8)	0.0082 (9)	0.0007 (9)
O6	0.0374 (9)	0.0500 (10)	0.0683 (10)	−0.0018 (8)	0.0103 (7)	0.0005 (8)

Geometric parameters (Å, º)

C1—C2	1.380 (3)	C12—C13	1.396 (3)
C1—C6	1.397 (3)	C12—C22	1.501 (3)
C1—C11	1.505 (3)	C13—C14	1.380 (3)
C2—C3	1.388 (3)	C13—H13	0.9300
C2—H2	0.9300	C14—C15	1.371 (3)
C3—C4	1.386 (3)	C14—H14	0.9300
C3—C7	1.439 (3)	C15—O6	1.375 (2)
C4—C5	1.375 (3)	C15—C16	1.381 (3)
C4—O3	1.377 (2)	C16—C17	1.396 (3)
C5—C6	1.381 (3)	C16—C18	1.441 (3)

C5—H5	0.9300	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.340 (3)
C7—C8	1.336 (3)	C18—C20	1.490 (3)
C7—C9	1.490 (3)	C19—O6	1.380 (2)
C8—O3	1.377 (3)	C19—H19	0.9300
C8—H8	0.9300	C20—C21	1.483 (3)
C9—C10	1.488 (3)	C20—H20A	0.9700
C9—H9A	0.9700	C20—H20B	0.9700
C9—H9B	0.9700	C21—O5	1.213 (2)
C10—O2	1.216 (2)	C21—O4	1.319 (2)
C10—O1	1.307 (3)	C22—H22A	0.9600
C11—H11A	0.9600	C22—H22B	0.9600
C11—H11B	0.9600	C22—H22C	0.9600
C11—H11C	0.9600	O1—H1A	0.8200
C12—C17	1.384 (3)	O4—H4A	0.8200

C2—C1—C6	119.0 (2)	C13—C12—C22	119.7 (2)
C2—C1—C11	121.14 (19)	C14—C13—C12	122.7 (2)
C6—C1—C11	119.8 (2)	C14—C13—H13	118.7
C1—C2—C3	119.95 (19)	C12—C13—H13	118.7
C1—C2—H2	120.0	C15—C14—C13	116.2 (2)
C3—C2—H2	120.0	C15—C14—H14	121.9
C4—C3—C2	118.60 (19)	C13—C14—H14	121.9
C4—C3—C7	106.12 (18)	C14—C15—O6	126.0 (2)
C2—C3—C7	135.3 (2)	C14—C15—C16	123.9 (2)
C5—C4—O3	126.13 (19)	O6—C15—C16	110.04 (19)
C5—C4—C3	123.7 (2)	C15—C16—C17	118.54 (19)
O3—C4—C3	110.20 (18)	C15—C16—C18	106.53 (18)
C4—C5—C6	116.0 (2)	C17—C16—C18	134.85 (19)
C4—C5—H5	122.0	C12—C17—C16	119.64 (19)
C6—C5—H5	122.0	C12—C17—H17	120.2
C5—C6—C1	122.8 (2)	C16—C17—H17	120.2
C5—C6—H6	118.6	C19—C18—C16	105.42 (18)
C1—C6—H6	118.6	C19—C18—C20	130.66 (19)
C8—C7—C3	105.67 (19)	C16—C18—C20	123.91 (18)
C8—C7—C9	130.2 (2)	C18—C19—O6	112.70 (19)
C3—C7—C9	124.08 (19)	C18—C19—H19	123.6
C7—C8—O3	113.0 (2)	O6—C19—H19	123.6
C7—C8—H8	123.5	C21—C20—C18	117.34 (18)
O3—C8—H8	123.5	C21—C20—H20A	108.0
C10—C9—C7	117.23 (19)	C18—C20—H20A	108.0
C10—C9—H9A	108.0	C21—C20—H20B	108.0
C7—C9—H9A	108.0	C18—C20—H20B	108.0
C10—C9—H9B	108.0	H20A—C20—H20B	107.2
C7—C9—H9B	108.0	O5—C21—O4	122.4 (2)
H9A—C9—H9B	107.2	O5—C21—C20	125.2 (2)
O2—C10—O1	122.7 (2)	O4—C21—C20	112.35 (19)
O2—C10—C9	124.7 (2)	C12—C22—H22A	109.5

O1—C10—C9	112.5 (2)	C12—C22—H22B	109.5
C1—C11—H11A	109.5	H22A—C22—H22B	109.5
C1—C11—H11B	109.5	C12—C22—H22C	109.5
H11A—C11—H11B	109.5	H22A—C22—H22C	109.5
C1—C11—H11C	109.5	H22B—C22—H22C	109.5
H11A—C11—H11C	109.5	C10—O1—H1A	109.5
H11B—C11—H11C	109.5	C4—O3—C8	105.01 (16)
C17—C12—C13	119.0 (2)	C21—O4—H4A	109.5
C17—C12—C22	121.3 (2)	C15—O6—C19	105.31 (16)

C6—C1—C2—C3	−0.2 (3)	C13—C14—C15—O6	176.28 (18)
C11—C1—C2—C3	179.80 (17)	C13—C14—C15—C16	−0.5 (3)
C1—C2—C3—C4	0.3 (3)	C14—C15—C16—C17	−0.6 (3)
C1—C2—C3—C7	−179.0 (2)	O6—C15—C16—C17	−177.81 (16)
C2—C3—C4—C5	−0.1 (3)	C14—C15—C16—C18	176.63 (19)
C7—C3—C4—C5	179.39 (19)	O6—C15—C16—C18	−0.6 (2)
C2—C3—C4—O3	−179.20 (16)	C13—C12—C17—C16	0.1 (3)
C7—C3—C4—O3	0.3 (2)	C22—C12—C17—C16	−179.93 (18)
O3—C4—C5—C6	178.69 (18)	C15—C16—C17—C12	0.8 (3)
C3—C4—C5—C6	−0.2 (3)	C18—C16—C17—C12	−175.5 (2)
C4—C5—C6—C1	0.4 (3)	C15—C16—C18—C19	0.0 (2)
C2—C1—C6—C5	−0.2 (3)	C17—C16—C18—C19	176.6 (2)
C11—C1—C6—C5	179.81 (19)	C15—C16—C18—C20	−178.94 (17)
C4—C3—C7—C8	−0.4 (2)	C17—C16—C18—C20	−2.4 (3)
C2—C3—C7—C8	179.0 (2)	C16—C18—C19—O6	0.6 (2)
C4—C3—C7—C9	179.34 (19)	C20—C18—C19—O6	179.43 (18)
C2—C3—C7—C9	−1.3 (4)	C19—C18—C20—C21	−2.4 (3)
C3—C7—C8—O3	0.3 (2)	C16—C18—C20—C21	176.29 (17)
C9—C7—C8—O3	−179.4 (2)	C18—C20—C21—O5	4.1 (3)
C8—C7—C9—C10	8.2 (4)	C18—C20—C21—O4	−176.54 (17)
C3—C7—C9—C10	−171.4 (2)	C5—C4—O3—C8	−179.2 (2)
C7—C9—C10—O2	−17.1 (4)	C3—C4—O3—C8	−0.2 (2)
C7—C9—C10—O1	164.1 (2)	C7—C8—O3—C4	−0.1 (2)
C17—C12—C13—C14	−1.3 (3)	C14—C15—O6—C19	−176.2 (2)
C22—C12—C13—C14	178.77 (19)	C16—C15—O6—C19	0.9 (2)
C12—C13—C14—C15	1.5 (3)	C18—C19—O6—C15	−0.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O5^{i}	0.82	1.83	2.650 (2)	176
O4—H4*A*···O2^{ii}	0.82	1.90	2.715 (2)	179
C8—H8···O2	0.93	2.29	2.855 (3)	118
C19—H19···O5	0.93	2.29	2.843 (3)	118

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