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2-(6-Methyl-1-benzofuran-3-yl)acetic acid

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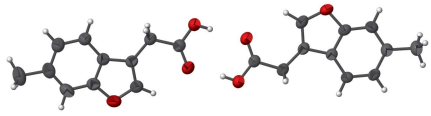
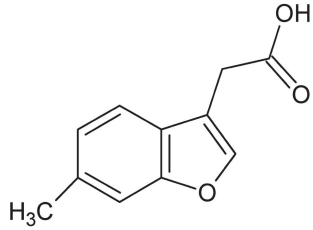
The asymmetric unit of the title compound, $C_{11}H_{10}O_3$, contains two crystallographically independent molecules (*A* and *B*) with nearly matching conformations. Both molecules are almost planar [r.m.s. overlay fit for the non-hydrogen atoms = 0.011 (1) Å] and in each molecule there is a short intramolecular C—H···O contact. In both molecules, the OH group of the acetic acid residue occupies a position approximately antiperiplanar to the C atom of the heterocycle. In the crystal, the two molecules are linked by a pair of O—H···O hydrogen bonds, enclosing an $R_2^2(8)$ ring motif and forming an *A*–*B* dimer. The dimers are linked by C—H···π interactions, forming columns along the [010] direction.

3D view



Chemical scheme



Structure description

Benzofuran derivatives have occupied an important place among various heterocycles by virtue of their involvement in medicinal chemistry and drug discovery (Hiremathad *et al.*, 2015). Carboxylic acids such as arylalkanoic acids exhibit interesting anti-inflammatory, analgesic and antipyretic properties, and so have been in wide clinical use for a number of years (Basanagouda *et al.* 2015).

The asymmetric unit of the title compound contains two crystallographically independent molecules (*A* = C1–C11/O1–O3 and *B* = C12–C22/O4–O6), which are almost identical (Fig. 1). Both molecules are almost planar with an r.m.s. overlay fit for the non-hydrogen atoms of 0.011 (1) Å. In each molecule there is a short intramolecular C—H···O contact present (Table 1). The bond lengths and angles of the title molecules are close to those observed for similar structures, *viz*. 2-(5-methoxy-1-benzofuran-3-yl)acetic

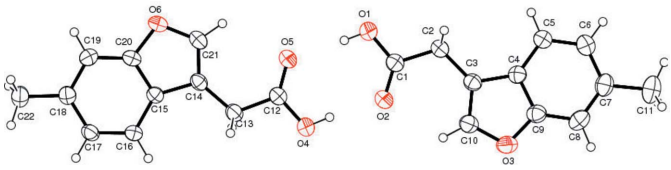


Figure 1
The molecular structure of the two independent molecules of the title compound, with atom labelling and 40% probability displacement ellipsoids. Figure 1 should show the O—H···O hydrogen bonds

acid (Gowda *et al.*, 2015) and 2-(5-methyl-1-benzofuran-3-yl)acetic acid (Ramprasad *et al.*, 2016).

In the crystal, the molecules are linked by a pair of O—H···O hydrogen bonds, enclosing an $R_2^2(8)$, ring motif and forming an *A*–*B* dimer (Fig. 2 and Table 1). The dimers are linked by C—H···π interactions forming columns along the [010] direction; see Table 1.

Synthesis and crystallization

The title compound was synthesized according to a reported procedure (Basanagouda *et al.*, 2015). 7-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 cooled, neutralized with 1 *M* HCl and the obtained product was filtered and dried. Pale-yellow block-like crystals were obtained by recrystallization from an ethanol and ethyl acetate solvent mixture by slow evaporation (m.p. 378–379 K).

Refinement

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

Acknowledgements

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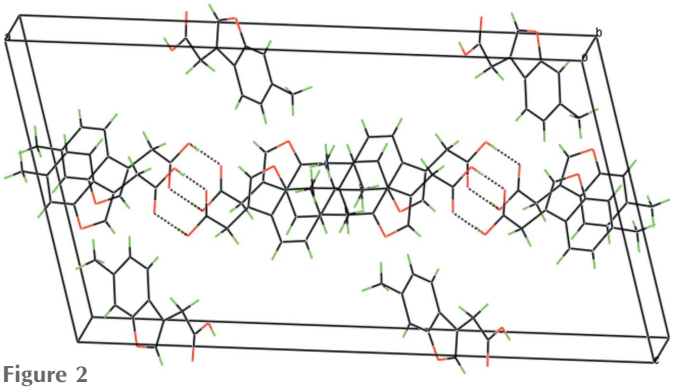

Figure 2
The crystal packing of the title compound, viewed along the *b* axis. The hydrogen bonds are shown as dashed lines (see Table 1).

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

*Cg*1 and *Cg*2 are the centroid of rings C4–C9 and C15–C20, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O5	0.82	1.90	2.7144 (15)	174
O4—H4···O2	0.82	1.83	2.6432 (15)	175
C10—H10···O2	0.93	2.25	2.813 (2)	118
C21—H21···O5	0.93	2.37	2.916 (2)	117
C2—H2*A*···*Cg*1^{i}	0.97	2.88	3.5629 (18)	128
C11—H11*A*···*Cg*1^{ii}	0.96	2.95	3.733 (2)	140
C13—H13*B*···*Cg*2^{ii}	0.97	2.86	3.5233 (17)	126
C22—H22*C*···*Cg*2^{i}	0.96	2.77	3.6955 (18)	162

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

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)	26.2392 (8), 5.1197 (1), 14.2546 (4)
β (°)	103.826 (1)
V (Å^3)	1859.43 (9)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.10
Crystal size (mm)	0.30 × 0.25 × 0.25
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.95, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41449, 3665, 2898
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.039, 0.115, 1.02
No. of reflections	3665
No. of parameters	257
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.19

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

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full crystallographic data

IUCrData (2016). **1**, x161434 [doi:10.1107/S2414314616014346]

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(I)

Crystal data

$C_{11}H_{10}O_3$
M_r = 190.19
Monoclinic, $P2_1/c$
a = 26.2392 (8) Å
b = 5.1197 (1) Å
c = 14.2546 (4) Å
β = 103.826 (1)°
V = 1859.43 (9) Å^3
Z = 8
$F(000)$ = 800
D_x = 1.359 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9885 reflections
θ = 2.9–25.3°
μ = 0.10 mm^{-1}
T = 296 K
Block, pale-yellow
0.30 × 0.25 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: Sealed tube
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.95, T_{max} = 0.98
41449 measured reflections
3665 independent reflections
2898 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.0°, θ_{min} = 2.4°
h = −32→32
k = −6→6
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.115
S = 1.02
3665 reflections
257 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
$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 0.5754P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.27076 (6)	0.7110 (3)	0.91891 (11)	0.0411 (4)
C2	0.29455 (6)	0.9059 (3)	0.86353 (11)	0.0450 (4)
H2A	0.3111	0.8109	0.8198	0.054*
H2B	0.2664	1.0089	0.8242	0.054*
C3	0.33414 (6)	1.0892 (3)	0.92134 (10)	0.0402 (4)
C4	0.36445 (6)	1.2734 (3)	0.88026 (11)	0.0420 (4)
C5	0.36823 (7)	1.3405 (4)	0.78736 (12)	0.0535 (4)
H5	0.3472	1.2593	0.7334	0.064*
C6	0.40388 (7)	1.5306 (4)	0.77748 (13)	0.0596 (5)
H6	0.4065	1.5762	0.7156	0.072*
C7	0.43625 (7)	1.6574 (4)	0.85653 (14)	0.0540 (4)
C8	0.43251 (7)	1.5924 (4)	0.94871 (14)	0.0554 (5)
H8	0.4533	1.6738	1.0028	0.067*
C9	0.39674 (6)	1.4024 (4)	0.95759 (11)	0.0469 (4)
C10	0.35008 (7)	1.1210 (4)	1.01690 (12)	0.0508 (4)
H10	0.3368	1.0255	1.0613	0.061*
C11	0.47501 (8)	1.8610 (4)	0.84131 (18)	0.0741 (6)
H11A	0.4714	2.0151	0.8775	0.111*
H11B	0.4683	1.9036	0.7739	0.111*
H11C	0.5100	1.7938	0.8628	0.111*
O1	0.23573 (5)	0.5612 (2)	0.86242 (8)	0.0542 (3)
H1	0.2237	0.4577	0.8955	0.081*
O2	0.28234 (5)	0.6905 (2)	1.00640 (8)	0.0518 (3)
O3	0.38825 (5)	1.3103 (3)	1.04283 (8)	0.0594 (3)
C12	0.21368 (6)	0.1683 (3)	1.05349 (11)	0.0386 (3)
C13	0.19482 (6)	−0.0334 (3)	1.11280 (10)	0.0419 (4)
H13A	0.2247	−0.1402	1.1435	0.050*
H13B	0.1831	0.0563	1.1638	0.050*
C14	0.15189 (6)	−0.2120 (3)	1.06360 (10)	0.0374 (3)
C15	0.12797 (6)	−0.4013 (3)	1.11542 (10)	0.0350 (3)
C16	0.13567 (6)	−0.4802 (3)	1.21139 (10)	0.0394 (3)
H16	0.1619	−0.4053	1.2595	0.047*
C17	0.10345 (6)	−0.6724 (3)	1.23336 (10)	0.0413 (4)
H17	0.1087	−0.7270	1.2972	0.050*
C18	0.06324 (6)	−0.7879 (3)	1.16331 (11)	0.0402 (3)
C19	0.05549 (6)	−0.7099 (3)	1.06785 (11)	0.0453 (4)
H19	0.0290	−0.7826	1.0197	0.054*
C20	0.08840 (6)	−0.5213 (3)	1.04675 (10)	0.0409 (4)
C21	0.12600 (7)	−0.2342 (4)	0.97102 (11)	0.0498 (4)
H21	0.1336	−0.1348	0.9214	0.060*
C22	0.02904 (7)	−0.9954 (3)	1.19135 (13)	0.0508 (4)
H22A	−0.0071	−0.9579	1.1620	0.076*
H22B	0.0343	−0.9980	1.2603	0.076*
H22C	0.0381	−1.1626	1.1695	0.076*
O4	0.24869 (4)	0.3244 (2)	1.10770 (8)	0.0502 (3)

H4	0.2582	0.4340	1.0735	0.075*
O5	0.19955 (5)	0.1894 (2)	0.96586 (8)	0.0491 (3)
O6	0.08679 (5)	−0.4203 (3)	0.95682 (7)	0.0548 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0426 (8)	0.0394 (8)	0.0417 (8)	0.0048 (7)	0.0105 (7)	0.0023 (7)
C2	0.0506 (9)	0.0463 (9)	0.0383 (8)	−0.0032 (7)	0.0110 (7)	0.0034 (7)
C3	0.0392 (8)	0.0435 (8)	0.0381 (8)	0.0042 (7)	0.0095 (6)	0.0026 (6)
C4	0.0398 (8)	0.0444 (9)	0.0418 (8)	0.0015 (7)	0.0095 (6)	−0.0005 (7)
C5	0.0582 (10)	0.0605 (11)	0.0415 (9)	−0.0127 (9)	0.0113 (8)	0.0008 (8)
C6	0.0613 (11)	0.0670 (12)	0.0530 (10)	−0.0115 (10)	0.0185 (9)	0.0044 (9)
C7	0.0424 (9)	0.0512 (10)	0.0699 (12)	−0.0024 (8)	0.0167 (8)	0.0000 (9)
C8	0.0428 (9)	0.0594 (11)	0.0613 (11)	−0.0052 (8)	0.0068 (8)	−0.0118 (9)
C9	0.0409 (8)	0.0555 (10)	0.0435 (9)	0.0017 (7)	0.0084 (7)	−0.0018 (7)
C10	0.0489 (9)	0.0616 (11)	0.0413 (8)	−0.0057 (8)	0.0096 (7)	0.0023 (8)
C11	0.0583 (12)	0.0636 (13)	0.1043 (17)	−0.0143 (10)	0.0275 (11)	0.0002 (12)
O1	0.0595 (7)	0.0548 (7)	0.0449 (6)	−0.0142 (6)	0.0061 (5)	0.0064 (5)
O2	0.0627 (7)	0.0525 (7)	0.0401 (6)	−0.0085 (6)	0.0123 (5)	0.0049 (5)
O3	0.0568 (7)	0.0776 (9)	0.0407 (6)	−0.0113 (7)	0.0057 (5)	−0.0041 (6)
C12	0.0412 (8)	0.0369 (8)	0.0393 (8)	0.0051 (6)	0.0126 (6)	0.0023 (6)
C13	0.0520 (9)	0.0393 (8)	0.0368 (8)	−0.0002 (7)	0.0151 (7)	0.0016 (6)
C14	0.0448 (8)	0.0354 (8)	0.0349 (7)	0.0048 (6)	0.0155 (6)	0.0017 (6)
C15	0.0386 (7)	0.0342 (7)	0.0340 (7)	0.0037 (6)	0.0119 (6)	−0.0009 (6)
C16	0.0436 (8)	0.0436 (8)	0.0312 (7)	−0.0017 (7)	0.0093 (6)	−0.0021 (6)
C17	0.0502 (9)	0.0441 (9)	0.0320 (7)	−0.0005 (7)	0.0144 (6)	0.0012 (6)
C18	0.0433 (8)	0.0374 (8)	0.0433 (8)	0.0017 (7)	0.0171 (7)	−0.0024 (6)
C19	0.0460 (9)	0.0474 (9)	0.0406 (8)	−0.0061 (7)	0.0065 (7)	−0.0055 (7)
C20	0.0468 (8)	0.0456 (9)	0.0302 (7)	0.0031 (7)	0.0089 (6)	0.0015 (6)
C21	0.0604 (10)	0.0518 (10)	0.0387 (8)	−0.0042 (8)	0.0148 (7)	0.0087 (7)
C22	0.0545 (10)	0.0444 (9)	0.0579 (10)	−0.0066 (8)	0.0222 (8)	−0.0023 (8)
O4	0.0555 (7)	0.0508 (7)	0.0439 (6)	−0.0107 (6)	0.0110 (5)	0.0048 (5)
O5	0.0591 (7)	0.0481 (7)	0.0401 (6)	−0.0065 (6)	0.0118 (5)	0.0067 (5)
O6	0.0644 (7)	0.0654 (8)	0.0308 (6)	−0.0123 (6)	0.0041 (5)	0.0061 (5)

Geometric parameters (Å, º)

C1—O2	1.2156 (18)	C12—O5	1.2199 (17)
C1—O1	1.3143 (19)	C12—O4	1.3195 (19)
C1—C2	1.498 (2)	C12—C13	1.492 (2)
C2—C3	1.493 (2)	C13—C14	1.490 (2)
C2—H2A	0.9700	C13—H13A	0.9700
C2—H2B	0.9700	C13—H13B	0.9700
C3—C10	1.336 (2)	C14—C21	1.337 (2)
C3—C4	1.445 (2)	C14—C15	1.449 (2)
C4—C9	1.387 (2)	C15—C20	1.389 (2)
C4—C5	1.394 (2)	C15—C16	1.3939 (19)

C5—C6	1.380 (2)	C16—C17	1.381 (2)
C5—H5	0.9300	C16—H16	0.9300
C6—C7	1.398 (3)	C17—C18	1.399 (2)
C6—H6	0.9300	C17—H17	0.9300
C7—C8	1.381 (3)	C18—C19	1.386 (2)
C7—C11	1.508 (3)	C18—C22	1.505 (2)
C8—C9	1.378 (2)	C19—C20	1.376 (2)
C8—H8	0.9300	C19—H19	0.9300
C9—O3	1.3703 (19)	C20—O6	1.3736 (17)
C10—O3	1.379 (2)	C21—O6	1.381 (2)
C10—H10	0.9300	C21—H21	0.9300
C11—H11A	0.9600	C22—H22A	0.9600
C11—H11B	0.9600	C22—H22B	0.9600
C11—H11C	0.9600	C22—H22C	0.9600
O1—H1	0.8200	O4—H4	0.8200

O2—C1—O1	123.02 (15)	O5—C12—O4	123.00 (14)
O2—C1—C2	124.38 (15)	O5—C12—C13	125.51 (14)
O1—C1—C2	112.59 (13)	O4—C12—C13	111.48 (12)
C3—C2—C1	116.77 (13)	C14—C13—C12	118.29 (13)
C3—C2—H2A	108.1	C14—C13—H13A	107.7
C1—C2—H2A	108.1	C12—C13—H13A	107.7
C3—C2—H2B	108.1	C14—C13—H13B	107.7
C1—C2—H2B	108.1	C12—C13—H13B	107.7
H2A—C2—H2B	107.3	H13A—C13—H13B	107.1
C10—C3—C4	105.38 (14)	C21—C14—C15	105.47 (14)
C10—C3—C2	130.26 (15)	C21—C14—C13	131.71 (14)
C4—C3—C2	124.35 (13)	C15—C14—C13	122.78 (13)
C9—C4—C5	117.98 (15)	C20—C15—C16	118.18 (14)
C9—C4—C3	106.24 (14)	C20—C15—C14	106.17 (12)
C5—C4—C3	135.78 (15)	C16—C15—C14	135.65 (14)
C6—C5—C4	118.32 (16)	C17—C16—C15	118.42 (14)
C6—C5—H5	120.8	C17—C16—H16	120.8
C4—C5—H5	120.8	C15—C16—H16	120.8
C5—C6—C7	122.75 (17)	C16—C17—C18	122.52 (14)
C5—C6—H6	118.6	C16—C17—H17	118.7
C7—C6—H6	118.6	C18—C17—H17	118.7
C8—C7—C6	119.16 (17)	C19—C18—C17	119.20 (14)
C8—C7—C11	120.47 (18)	C19—C18—C22	120.47 (14)
C6—C7—C11	120.37 (18)	C17—C18—C22	120.33 (14)
C9—C8—C7	117.52 (16)	C20—C19—C18	117.67 (14)
C9—C8—H8	121.2	C20—C19—H19	121.2
C7—C8—H8	121.2	C18—C19—H19	121.2
O3—C9—C8	125.65 (16)	O6—C20—C19	125.98 (14)
O3—C9—C4	110.07 (15)	O6—C20—C15	110.01 (13)
C8—C9—C4	124.28 (16)	C19—C20—C15	123.99 (13)
C3—C10—O3	112.90 (15)	C14—C21—O6	112.83 (14)
C3—C10—H10	123.5	C14—C21—H21	123.6

O3—C10—H10	123.5	O6—C21—H21	123.6
C7—C11—H11A	109.5	C18—C22—H22A	109.5
C7—C11—H11B	109.5	C18—C22—H22B	109.5
H11A—C11—H11B	109.5	H22A—C22—H22B	109.5
C7—C11—H11C	109.5	C18—C22—H22C	109.5
H11A—C11—H11C	109.5	H22A—C22—H22C	109.5
H11B—C11—H11C	109.5	H22B—C22—H22C	109.5
C1—O1—H1	109.5	C12—O4—H4	109.5
C9—O3—C10	105.41 (12)	C20—O6—C21	105.51 (12)

O2—C1—C2—C3	−1.5 (2)	O5—C12—C13—C14	−5.5 (2)
O1—C1—C2—C3	178.84 (14)	O4—C12—C13—C14	175.09 (13)
C1—C2—C3—C10	−4.8 (3)	C12—C13—C14—C21	1.9 (3)
C1—C2—C3—C4	174.18 (14)	C12—C13—C14—C15	−175.21 (13)
C10—C3—C4—C9	−0.01 (18)	C21—C14—C15—C20	−0.51 (17)
C2—C3—C4—C9	−179.25 (15)	C13—C14—C15—C20	177.27 (14)
C10—C3—C4—C5	179.0 (2)	C21—C14—C15—C16	179.70 (17)
C2—C3—C4—C5	−0.2 (3)	C13—C14—C15—C16	−2.5 (3)
C9—C4—C5—C6	0.2 (3)	C20—C15—C16—C17	−0.4 (2)
C3—C4—C5—C6	−178.79 (18)	C14—C15—C16—C17	179.42 (15)
C4—C5—C6—C7	0.1 (3)	C15—C16—C17—C18	−0.7 (2)
C5—C6—C7—C8	−0.4 (3)	C16—C17—C18—C19	0.7 (2)
C5—C6—C7—C11	179.15 (18)	C16—C17—C18—C22	−179.62 (14)
C6—C7—C8—C9	0.4 (3)	C17—C18—C19—C20	0.3 (2)
C11—C7—C8—C9	−179.20 (16)	C22—C18—C19—C20	−179.35 (14)
C7—C8—C9—O3	178.90 (16)	C18—C19—C20—O6	179.90 (14)
C7—C8—C9—C4	0.0 (3)	C18—C19—C20—C15	−1.4 (2)
C5—C4—C9—O3	−179.32 (15)	C16—C15—C20—O6	−179.69 (13)
C3—C4—C9—O3	−0.06 (18)	C14—C15—C20—O6	0.48 (17)
C5—C4—C9—C8	−0.2 (3)	C16—C15—C20—C19	1.4 (2)
C3—C4—C9—C8	179.03 (16)	C14—C15—C20—C19	−178.39 (15)
C4—C3—C10—O3	0.08 (19)	C15—C14—C21—O6	0.37 (19)
C2—C3—C10—O3	179.25 (15)	C13—C14—C21—O6	−177.13 (15)
C8—C9—O3—C10	−178.97 (17)	C19—C20—O6—C21	178.57 (16)
C4—C9—O3—C10	0.11 (18)	C15—C20—O6—C21	−0.27 (18)
C3—C10—O3—C9	−0.12 (19)	C14—C21—O6—C20	−0.08 (19)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroid of rings C4–C9 and C15–C20, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O5	0.82	1.90	2.7144 (15)	174
O4—H4···O2	0.82	1.83	2.6432 (15)	175
C10—H10···O2	0.93	2.25	2.813 (2)	118
C21—H21···O5	0.93	2.37	2.916 (2)	117
C2—H2*A*···*Cg*1^{i}	0.97	2.88	3.5629 (18)	128
C11—H11*A*···*Cg*1^{ii}	0.96	2.95	3.733 (2)	140

C13—H13*B*···*Cg2*^{ii}	0.97	2.86	3.5233 (17)	126
C22—H22*C*···*Cg2*^{i}	0.96	2.77	3.6955 (18)	162

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