

Ethyl 3-hydroxybenzoate

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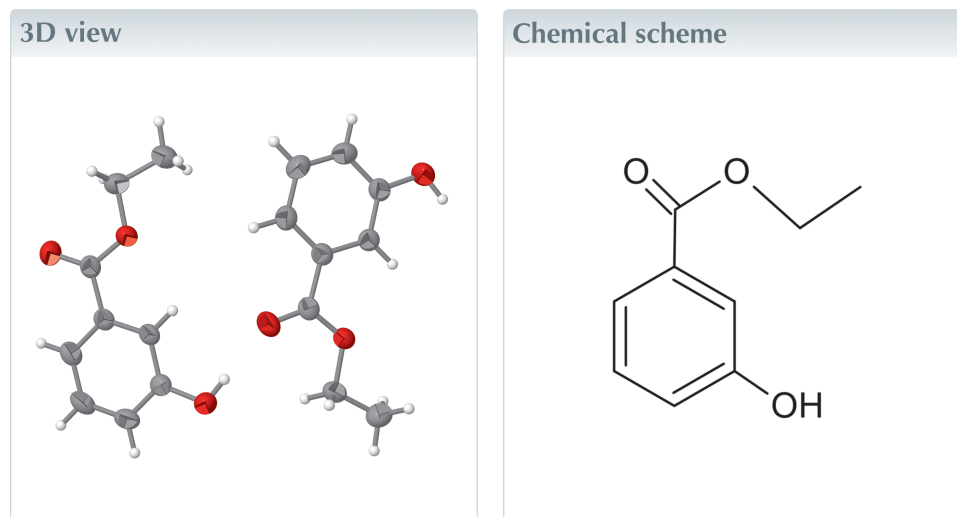
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Structural data: full structural data are available from iucrdata.iucr.org

The crystal of ethyl 3-hydroxybenzoate, $C_9H_{10}O_3$, comprises two independent molecules in the asymmetric unit. Each molecule is approximately planar with the ethyl group directed away from the carbonyl-O atom. The planarity is reflected in the phenyl-C—C—O—C(methylene) torsion angles of -179.40 (10) and 177.88 (11) $^\circ$, respectively. The greatest difference between the molecules is found in the relative orientations of the methyl groups as seen in the carboxylate-C—O—C—C(methyl) torsion angles of -178.76 (11) and -171.12 (13) $^\circ$, respectively. In the crystal, hydroxyl-O—H \cdots O(carbonyl) hydrogen-bonding occurs within almost planar chains along [100].



Structure description

The reaction of 3-hydroxybenzoic acid with ethanol yielded the title compound, ethyl 3-hydroxybenzoate, which has applications in organic synthesis and as a food preservative (Goretti *et al.*, 2009). The crystal structure report herein complements an undergraduate Organic Chemistry laboratory experiment (Hermann *et al.*, 2026), as detailed in Gutzwiller *et al.* (2026). The title compound crystallizes with two molecules in the asymmetric unit, Fig. 1. Each independent molecule is essentially planar as seen in the value of the C1₁—C7₁—O1₁—C8₁ torsion angle of -179.40 (10) $^\circ$. The equivalent value for the second independent molecule is 177.88 (11) $^\circ$. A small deviation in the orientation of the terminal methyl groups is noted: the C7₁—O1₁—C8₁—C9₁ torsion angle is -178.76 (11) $^\circ$ *cf.* C7₂—O1₂—C8₂—C9₂ of -171.12 (13) $^\circ$.

Hydrogen-bonding of the type hydroxyl-O—H \cdots O(carbonyl) is observed within approximately planar chains along the *a*-axis direction. The chains stack along the *b*-axis direction in an $\cdots ABA \cdots$ fashion. The hydrogen-bonding parameters are given in Table 1 and a view of the unit-cell contents is shown in Fig. 2.

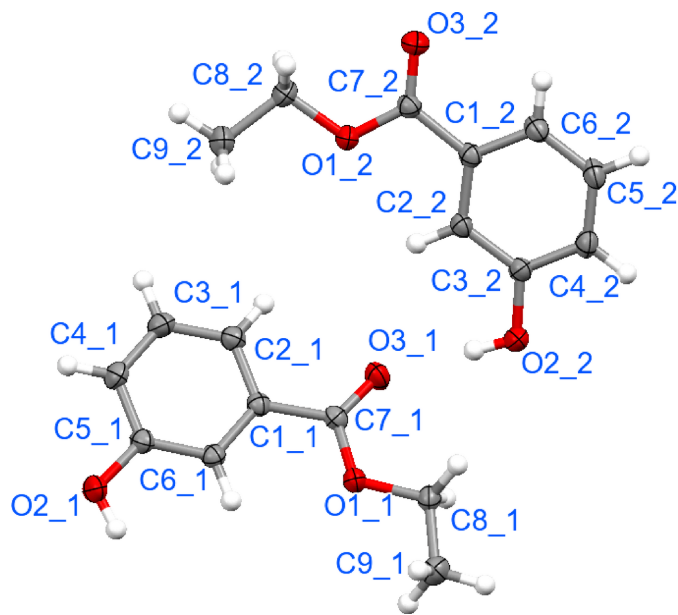


Figure 1
The molecular structures of the two independent molecules comprising the title compound showing atom labeling scheme and displacement ellipsoids at the 30% probability level.

Synthesis and crystallization

Referring to Fig. 3, the title compound was synthesized through a Fischer esterification. A mixture of 3-hydroxybenzoic acid (1.5 g), ethanol (10 ml) and concentrated sulfuric

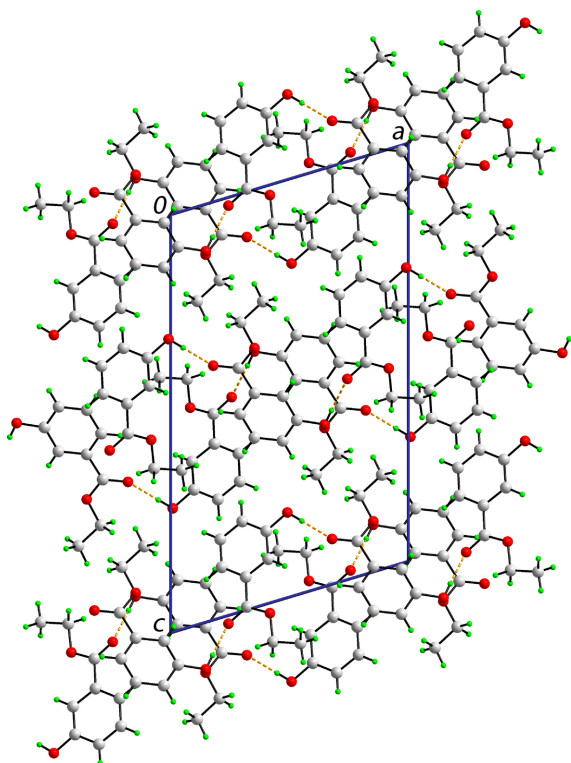


Figure 2
Molecular packing diagram viewed in projection down the *b* axis. Hydrogen-bonding interactions are shown as orange dashed lines.

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O2_1–H1_1···O3_2 ⁱ	0.87 (2)	1.88 (2)	2.7495 (15)	177 (2)
O2_2–H1_2···O3_1	0.84 (2)	1.93 (2)	2.7617 (14)	178.1 (14)

Symmetry code: (i) *x* + 1, *y*, *z*.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₉ H ₁₀ O ₃
<i>M_r</i>	166.17
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	248
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.8207 (8), 7.4541 (6), 19.9477 (15)
β (°)	106.776 (2)
<i>V</i> (Å ³)	1682.8 (2)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.10
Crystal size (mm)	0.6 × 0.4 × 0.4
Data collection	
Diffractometer	Bruker D8
Absorption correction	Multi-scan (SADAB; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.943, 0.962
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	42216, 4174, 3152
<i>R</i> _{int}	0.035
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.667
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.042, 0.129, 1.01
No. of reflections	4174
No. of parameters	225
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.19, -0.21

Computer programs: *APEX3* and *SAINT* (Bruker, 2019), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2019/3* (Sheldrick, 2015b) and *shelXle* (Hübschle *et al.*, 2011).

acid (1 ml) was refluxed in a 50 ml boiling flask for 1 h. The reaction mixture was allowed to cool, then a solution of 10% sodium carbonate was added until a pH of 8 was obtained. The solution was chilled in an ice-bath until a solid product was formed. The solid was isolated by vacuum filtration.

The yield of the crude product was 0.992 g (54.3%) with a melting point of 67.2°C. X-ray quality crystals were produced by dissolving the product into methanol, followed by adding an equal volume of hexanes. The solvent was allowed to evaporate over several days. A single-crystal was coated with NVH oil and mounted on a MiTeGen loop then cooled to 248 K for data collection.

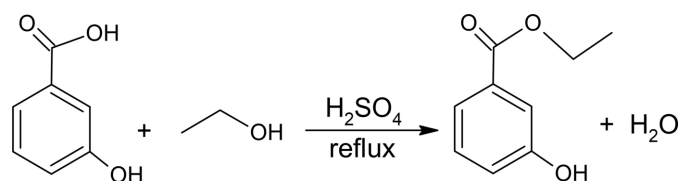


Figure 3
Reaction scheme for the title compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Owing to poor agreement, one reflection, *i.e.* 002, was omitted from the final cycles of refinement.

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full crystallographic data

IUCrData (2026). **11**, x260569 [https://doi.org/10.1107/S2414314626005699]

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Crystal data

$C_9H_{10}O_3$	$F(000) = 704$
$M_r = 166.17$	$D_x = 1.312 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 11.8207 (8) \text{ \AA}$	Cell parameters from 9996 reflections
$b = 7.4541 (6) \text{ \AA}$	$\theta = 2.9\text{--}28.2^\circ$
$c = 19.9477 (15) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$\beta = 106.776 (2)^\circ$	$T = 248 \text{ K}$
$V = 1682.8 (2) \text{ \AA}^3$	Block, colourless
$Z = 8$	$0.6 \times 0.4 \times 0.4 \text{ mm}$

Data collection

Bruker D8 diffractometer	42216 measured reflections
Radiation source: sealed tube	4174 independent reflections
Flat graphite monochromator	3152 reflections with $I > 2\sigma(I)$
Detector resolution: $7.391 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.035$
ω and ϕ scans	$\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (SADAB; Krause <i>et al.</i> , 2015)	$h = -15 \rightarrow 15$
$T_{\text{min}} = 0.943$, $T_{\text{max}} = 0.962$	$k = -9 \rightarrow 9$
	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.129$	$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.2243P]$
$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
4174 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
225 parameters	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
Primary atom site location: Intrinsic Phasing	

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1_1	0.91779 (7)	0.26186 (12)	0.52442 (4)	0.0429 (2)
O2_1	0.99117 (9)	0.39106 (17)	0.29620 (5)	0.0585 (3)
H1_1	1.0520 (18)	0.344 (3)	0.3269 (11)	0.088*
O3_1	0.74342 (8)	0.38538 (14)	0.51992 (5)	0.0521 (3)
C1_1	0.81601 (10)	0.40712 (16)	0.42054 (6)	0.0364 (3)
C2_1	0.71478 (11)	0.49152 (18)	0.37984 (7)	0.0436 (3)
H2_1	0.651122	0.514149	0.398019	0.052*
C3_1	0.70881 (12)	0.5419 (2)	0.31215 (7)	0.0502 (3)
H3_1	0.641020	0.600555	0.284399	0.060*
C4_1	0.80135 (12)	0.5069 (2)	0.28510 (7)	0.0506 (3)
H4_1	0.796059	0.541026	0.238929	0.061*
C5_1	0.90218 (11)	0.42163 (18)	0.32550 (6)	0.0422 (3)
C6_1	0.91060 (10)	0.37347 (16)	0.39395 (6)	0.0374 (3)
H6_1	0.979587	0.318581	0.422117	0.045*
C7_1	0.82072 (10)	0.35279 (16)	0.49288 (6)	0.0378 (3)
C8_1	0.93052 (11)	0.20084 (19)	0.59518 (6)	0.0438 (3)
H8A_1	0.866292	0.118519	0.595989	0.053*
H8B_1	0.928780	0.302882	0.625844	0.053*
C9_1	1.04619 (13)	0.1077 (2)	0.61868 (8)	0.0579 (4)
H9A_1	1.058095	0.061953	0.665739	0.087*
H9B_1	1.108907	0.191394	0.618440	0.087*
H9C_1	1.047199	0.008842	0.587237	0.087*
O1_2	0.35295 (7)	0.31978 (14)	0.37940 (4)	0.0462 (2)
O2_2	0.64798 (8)	0.20855 (16)	0.61254 (5)	0.0547 (3)
H1_2	0.6765 (17)	0.260 (3)	0.5839 (10)	0.082*
O3_2	0.17933 (8)	0.23070 (15)	0.39172 (5)	0.0535 (3)
C1_2	0.35271 (10)	0.19414 (16)	0.48736 (6)	0.0368 (3)
C2_2	0.47221 (10)	0.23244 (16)	0.51480 (6)	0.0374 (3)
H2_2	0.512709	0.295759	0.488075	0.045*
C3_2	0.53107 (10)	0.17608 (17)	0.58216 (6)	0.0394 (3)
C4_2	0.47110 (12)	0.08158 (19)	0.62121 (7)	0.0466 (3)
H4_2	0.511232	0.043009	0.666734	0.056*
C5_2	0.35258 (13)	0.0443 (2)	0.59319 (7)	0.0510 (3)
H5_2	0.312368	-0.020393	0.619708	0.061*
C6_2	0.29236 (12)	0.10108 (19)	0.52656 (7)	0.0453 (3)
H6_2	0.211274	0.076893	0.507945	0.054*
C7_2	0.28568 (11)	0.24977 (17)	0.41548 (6)	0.0392 (3)
C8_2	0.29433 (12)	0.3718 (2)	0.30758 (7)	0.0522 (3)
H8A_2	0.242762	0.475260	0.306633	0.063*
H8B_2	0.246061	0.272506	0.282369	0.063*
C9_2	0.38821 (14)	0.4186 (3)	0.27424 (8)	0.0666 (5)
H9A_2	0.351992	0.451530	0.225729	0.100*
H9B_2	0.439587	0.315993	0.276354	0.100*
H9C_2	0.434153	0.518786	0.298951	0.100*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1_1	0.0392 (5)	0.0542 (5)	0.0374 (5)	0.0024 (4)	0.0143 (4)	0.0068 (4)
O2_1	0.0482 (6)	0.0939 (8)	0.0373 (5)	0.0085 (5)	0.0187 (4)	0.0022 (5)
O3_1	0.0495 (5)	0.0623 (6)	0.0526 (6)	0.0097 (4)	0.0277 (5)	0.0096 (4)
C1_1	0.0369 (6)	0.0366 (6)	0.0361 (6)	-0.0044 (5)	0.0113 (5)	-0.0022 (5)
C2_1	0.0371 (6)	0.0491 (7)	0.0453 (7)	0.0013 (5)	0.0130 (5)	-0.0008 (6)
C3_1	0.0407 (7)	0.0624 (9)	0.0427 (7)	0.0048 (6)	0.0045 (5)	0.0028 (6)
C4_1	0.0487 (7)	0.0680 (9)	0.0328 (6)	0.0002 (7)	0.0079 (5)	0.0011 (6)
C5_1	0.0380 (6)	0.0546 (7)	0.0349 (6)	-0.0036 (5)	0.0117 (5)	-0.0058 (5)
C6_1	0.0352 (6)	0.0406 (6)	0.0359 (6)	-0.0016 (5)	0.0096 (5)	-0.0022 (5)
C7_1	0.0369 (6)	0.0370 (6)	0.0411 (6)	-0.0030 (5)	0.0139 (5)	-0.0008 (5)
C8_1	0.0457 (7)	0.0507 (7)	0.0361 (6)	-0.0046 (6)	0.0136 (5)	0.0046 (5)
C9_1	0.0536 (8)	0.0662 (9)	0.0516 (8)	0.0054 (7)	0.0116 (7)	0.0112 (7)
O1_2	0.0380 (5)	0.0658 (6)	0.0349 (5)	-0.0016 (4)	0.0105 (4)	0.0069 (4)
O2_2	0.0388 (5)	0.0853 (8)	0.0390 (5)	0.0031 (5)	0.0094 (4)	0.0112 (5)
O3_2	0.0365 (5)	0.0722 (7)	0.0497 (6)	-0.0054 (4)	0.0092 (4)	0.0034 (5)
C1_2	0.0387 (6)	0.0398 (6)	0.0349 (6)	0.0009 (5)	0.0154 (5)	-0.0035 (5)
C2_2	0.0381 (6)	0.0432 (6)	0.0347 (6)	0.0031 (5)	0.0163 (5)	0.0015 (5)
C3_2	0.0379 (6)	0.0470 (7)	0.0352 (6)	0.0062 (5)	0.0135 (5)	-0.0007 (5)
C4_2	0.0562 (8)	0.0525 (8)	0.0343 (6)	0.0053 (6)	0.0183 (6)	0.0047 (6)
C5_2	0.0595 (8)	0.0568 (8)	0.0440 (7)	-0.0099 (7)	0.0266 (6)	0.0019 (6)
C6_2	0.0441 (7)	0.0526 (8)	0.0430 (7)	-0.0088 (6)	0.0185 (5)	-0.0048 (6)
C7_2	0.0367 (6)	0.0443 (6)	0.0386 (6)	-0.0003 (5)	0.0139 (5)	-0.0034 (5)
C8_2	0.0469 (7)	0.0711 (9)	0.0354 (7)	-0.0011 (7)	0.0069 (6)	0.0061 (6)
C9_2	0.0590 (9)	0.0982 (13)	0.0464 (8)	0.0049 (9)	0.0212 (7)	0.0156 (8)

Geometric parameters (\AA , $^\circ$)

O1_1—C7_1	1.3248 (15)	O1_2—C7_2	1.3239 (14)
O1_1—C8_1	1.4489 (14)	O1_2—C8_2	1.4525 (15)
O2_1—C5_1	1.3620 (15)	O2_2—C3_2	1.3609 (15)
O3_1—C7_1	1.2121 (14)	O3_2—C7_2	1.2171 (15)
C1_1—C2_1	1.3878 (17)	C1_2—C6_2	1.3870 (17)
C1_1—C6_1	1.3918 (16)	C1_2—C2_2	1.3892 (17)
C1_1—C7_1	1.4842 (17)	C1_2—C7_2	1.4831 (18)
C2_1—C3_1	1.3835 (19)	C2_2—C3_2	1.3879 (17)
C3_1—C4_1	1.3773 (19)	C3_2—C4_2	1.3872 (18)
C4_1—C5_1	1.3855 (19)	C4_2—C5_2	1.378 (2)
C5_1—C6_1	1.3873 (17)	C5_2—C6_2	1.3807 (19)
C8_1—C9_1	1.484 (2)	C8_2—C9_2	1.4905 (19)
C7_1—O1_1—C8_1	117.09 (9)	C7_2—O1_2—C8_2	116.81 (10)
C2_1—C1_1—C6_1	120.70 (11)	C6_2—C1_2—C2_2	120.70 (12)
C2_1—C1_1—C7_1	118.46 (11)	C6_2—C1_2—C7_2	117.82 (11)
C6_1—C1_1—C7_1	120.83 (11)	C2_2—C1_2—C7_2	121.48 (11)
C3_1—C2_1—C1_1	119.11 (11)	C3_2—C2_2—C1_2	119.21 (11)

C4_1—C3_1—C2_1	120.56 (13)	O2_2—C3_2—C4_2	117.27 (11)
C3_1—C4_1—C5_1	120.41 (12)	O2_2—C3_2—C2_2	122.56 (11)
O2_1—C5_1—C4_1	117.93 (11)	C4_2—C3_2—C2_2	120.18 (12)
O2_1—C5_1—C6_1	122.29 (12)	C5_2—C4_2—C3_2	119.93 (12)
C4_1—C5_1—C6_1	119.77 (12)	C4_2—C5_2—C6_2	120.66 (12)
C5_1—C6_1—C1_1	119.42 (11)	C5_2—C6_2—C1_2	119.33 (12)
O3_1—C7_1—O1_1	123.51 (11)	O3_2—C7_2—O1_2	123.32 (12)
O3_1—C7_1—C1_1	123.80 (11)	O3_2—C7_2—C1_2	123.18 (11)
O1_1—C7_1—C1_1	112.68 (10)	O1_2—C7_2—C1_2	113.49 (10)
O1_1—C8_1—C9_1	106.37 (11)	O1_2—C8_2—C9_2	107.34 (11)
C6_1—C1_1—C2_1—C3_1	0.08 (19)	C6_2—C1_2—C2_2—C3_2	0.13 (18)
C7_1—C1_1—C2_1—C3_1	-179.59 (12)	C7_2—C1_2—C2_2—C3_2	-179.47 (11)
C1_1—C2_1—C3_1—C4_1	0.8 (2)	C1_2—C2_2—C3_2—O2_2	179.98 (11)
C2_1—C3_1—C4_1—C5_1	-0.4 (2)	C1_2—C2_2—C3_2—C4_2	0.45 (18)
C3_1—C4_1—C5_1—O2_1	-179.71 (13)	O2_2—C3_2—C4_2—C5_2	-179.87 (12)
C3_1—C4_1—C5_1—C6_1	-0.9 (2)	C2_2—C3_2—C4_2—C5_2	-0.3 (2)
O2_1—C5_1—C6_1—C1_1	-179.45 (12)	C3_2—C4_2—C5_2—C6_2	-0.4 (2)
C4_1—C5_1—C6_1—C1_1	1.76 (19)	C4_2—C5_2—C6_2—C1_2	1.0 (2)
C2_1—C1_1—C6_1—C5_1	-1.37 (18)	C2_2—C1_2—C6_2—C5_2	-0.83 (19)
C7_1—C1_1—C6_1—C5_1	178.29 (11)	C7_2—C1_2—C6_2—C5_2	178.79 (12)
C8_1—O1_1—C7_1—O3_1	-0.51 (18)	C8_2—O1_2—C7_2—O3_2	-1.23 (19)
C8_1—O1_1—C7_1—C1_1	-179.40 (10)	C8_2—O1_2—C7_2—C1_2	177.88 (11)
C2_1—C1_1—C7_1—O3_1	-3.67 (19)	C6_2—C1_2—C7_2—O3_2	6.19 (19)
C6_1—C1_1—C7_1—O3_1	176.66 (12)	C2_2—C1_2—C7_2—O3_2	-174.20 (12)
C2_1—C1_1—C7_1—O1_1	175.22 (11)	C6_2—C1_2—C7_2—O1_2	-172.92 (11)
C6_1—C1_1—C7_1—O1_1	-4.45 (16)	C2_2—C1_2—C7_2—O1_2	6.69 (17)
C7_1—O1_1—C8_1—C9_1	-178.76 (11)	C7_2—O1_2—C8_2—C9_2	-171.12 (13)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2_1—H1_1...O3_2 ⁱ	0.87 (2)	1.88 (2)	2.7495 (15)	177 (2)
O2_2—H1_2...O3_1	0.84 (2)	1.93 (2)	2.7617 (14)	178.1 (14)

Symmetry code: (i) *x*+1, *y*, *z*.