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Butyl 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)propanoate

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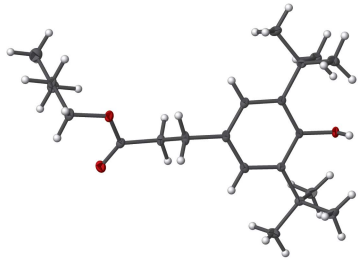
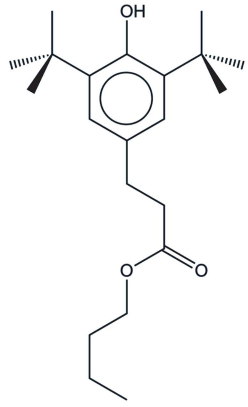
Millimeter-sized crystalline particles of butyl 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)propanoate, $C_{21}H_{34}O_3$, magnitudes larger than adherent particulate matter commonly observed during routine filter service inspections, were found in a commercial bus engine running on compressed methane biofuels and subjected to single-crystal XRD investigation. The structure is fully ordered and shows molecules in rather extended conformations being linked into chains by O—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

Multiple 0.7–2.0 mm agglomerates of translucent, spherically shaped, greyish white crystalline matter (Fig. 1) were found clustering a metal particle filter together with minor amounts of bituminous matter and inorganics. The particles were first observed during routine fuel filter inspections from a biofueled (compressed methane) bus engine. They expose well-defined transparent crystallites, some containing large two-phase gas–liquid fluid inclusions of 10–30 µm (Kihle *et al.*, 2012). Observations of trapped fluid inclusion gas bubble volume expansion during crystal dissolution when immersed in benzaldehyde at 22°C correspond to pressurized trapping conditions of 5–8 bars.

Subsequent analysis of a well-diffracting single crystal cut from one such agglomerate led to identification of the title compound (I).

The molecular structure of (I) [Fig. 2(*a*)] is fully ordered. A *trans* orientation for C1—C2—C3—C4 combined with a *gauche* orientation for O1—C18—C19—C20 (Table 1) puts the *n*-butyl group outside the plane of the aromatic ring [Fig. 2(*b*)]. Individual molecules are connected by hydrogen bonds (Table 2) into chains along the *b*-axis direction (Fig. 3).

Table 1
Selected torsion angles (°).

C18—O1—C1—C2	177.72 (7)	C1—O1—C18—C19	−108.05 (9)
O1—C1—C2—C3	53.83 (10)	O1—C18—C19—C20	64.77 (9)
C1—C2—C3—C4	178.11 (7)	C18—C19—C20—C21	180.00 (8)
C2—C3—C4—C5	−78.82 (10)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2^{i}	0.841 (13)	1.905 (13)	2.7399 (13)	172.1 (12)

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

The structure of the corresponding free acid was reported only recently (Jaivel *et al.*, 2015), a year after the methyl ester (Li *et al.*, 2014). Intermolecular interactions in crystals of the former are dominated by the formation of carboxylic acid dimers; the hydroxyl group is left without an apparent hydrogen-bond acceptor, while chains corresponding to those of (I) occur for the latter, although with much longer O···H distances of 2.51 Å compared to 1.905 (13) Å for (I) (Table 2).

The origin of the solid propionate in the filter probably (and ironically) stems from its use as a fuel additive for the inhi-

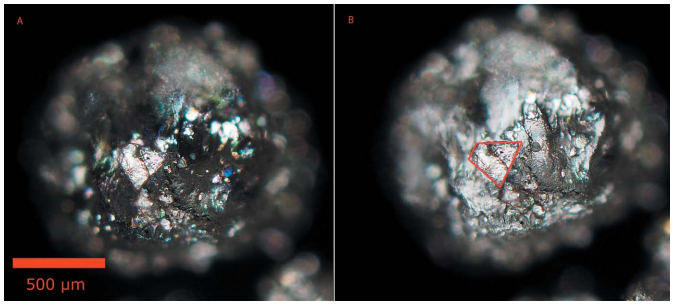


Figure 1
Optical microscopy images of a typical agglomerate particle under (*a*) cross- and (*b*) parallel-polarized transmitted light, revealing outlines of single crystallites (in red).

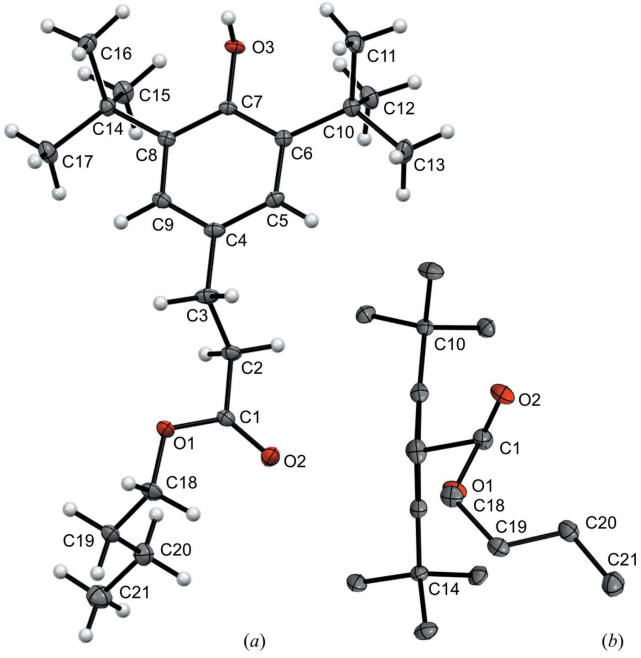


Figure 2
(*a*) The molecular structure of (I) at 100 K. Thermal displacement ellipsoids are shown at the 50% probability level. (*b*) Rotated view, H atoms excluded.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{34}O_3$
M_r	334.48
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	9.871 (4), 10.973 (5), 18.067 (7)
β (°)	91.908 (14)
V (Å^3)	1956.0 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.75 × 0.68 × 0.47
Data collection	
Diffractometer	Photon 100 CMOS detector, Bruker D8 Venture
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.917, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	43859, 6850, 5673
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.749
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.111, 1.03
No. of reflections	6850
No. of parameters	227
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.23

Computer programs: *APEX2* and *SAINT-Plus* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2008).

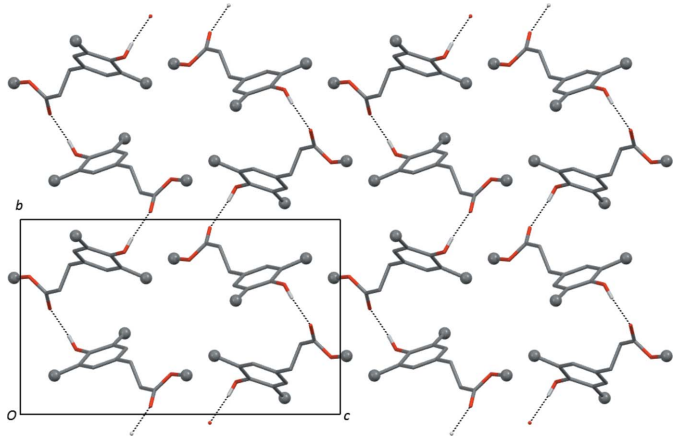


Figure 3
The unit cell and crystal packing viewed along the *a* axis. For clarity, only the hydroxylic H atoms have been included, while methyl and butyl groups are shown as small spheres. Hydrogen-bonded chains run along the vertical *b* axis.

bition of (organic) particle formation. We suspect that engine running conditions or additive concentrations have been off target.

Synthesis and crystallization

The investigated crystal was harvested from a fuel inlet particle filter of a biofuel bus engine.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

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full crystallographic data

IUCrData (2019). **4**, x190289 [https://doi.org/10.1107/S241431461900289X]

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Crystal data

$C_{21}H_{34}O_3$
M_r = 334.48
Monoclinic, $P2_1/c$
a = 9.871 (4) Å
b = 10.973 (5) Å
c = 18.067 (7) Å
β = 91.908 (14)°
V = 1956.0 (14) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.136 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9986 reflections
θ = 2.8–32.1°
μ = 0.07 mm^{-1}
T = 100 K
Block, colourless
0.75 × 0.68 × 0.47 mm

Data collection

Photon 100 CMOS detector, Bruker D8 Venture diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8.3 pixels mm^{-1}
Sets of exposures each taken over 0.5° ω rotation scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.917, T_{max} = 1.000
43859 measured reflections
6850 independent reflections
5673 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 32.2°, θ_{min} = 2.2°
h = −14→14
k = −16→16
l = −27→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.111
S = 1.03
6850 reflections
227 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.4869P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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. No restraints or constraints applied.
Normal anisotropic refinement, hydroxylic H atom refined isotropically, other H atoms in calculated positions, rotatable methyl groups.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.77265 (6)	0.79336 (6)	0.52808 (3)	0.01761 (13)
O2	0.84565 (6)	0.95653 (6)	0.59254 (4)	0.01949 (13)
O3	0.15240 (6)	0.66644 (6)	0.82531 (3)	0.01359 (12)
H3	0.1591 (12)	0.5997 (12)	0.8480 (7)	0.020*
C1	0.76186 (8)	0.87740 (7)	0.58083 (4)	0.01334 (14)
C2	0.63402 (8)	0.86147 (7)	0.62320 (4)	0.01460 (15)
H21	0.5548	0.8794	0.5900	0.018*
H22	0.6340	0.9209	0.6644	0.018*
C3	0.61960 (9)	0.73242 (8)	0.65463 (5)	0.01733 (16)
H31	0.6166	0.6733	0.6132	0.021*
H32	0.7004	0.7135	0.6865	0.021*
C4	0.49381 (8)	0.71708 (7)	0.69932 (4)	0.01388 (14)
C5	0.49123 (8)	0.75974 (7)	0.77168 (4)	0.01392 (14)
H51	0.5691	0.7997	0.7923	0.017*
C6	0.37796 (8)	0.74576 (7)	0.81499 (4)	0.01178 (14)
C7	0.26551 (7)	0.68355 (7)	0.78325 (4)	0.01101 (13)
C8	0.26160 (8)	0.64371 (7)	0.70921 (4)	0.01157 (13)
C9	0.37823 (8)	0.66210 (7)	0.66878 (4)	0.01338 (14)
H91	0.3784	0.6361	0.6186	0.016*
C10	0.37449 (8)	0.80074 (7)	0.89320 (4)	0.01368 (14)
C11	0.35803 (10)	0.70137 (8)	0.95237 (5)	0.02031 (17)
H111	0.2682	0.6640	0.9462	0.030*
H112	0.3675	0.7379	1.0018	0.030*
H113	0.4279	0.6389	0.9468	0.030*
C12	0.25809 (9)	0.89393 (8)	0.89601 (5)	0.01847 (16)
H121	0.2670	0.9535	0.8561	0.028*
H122	0.2621	0.9360	0.9439	0.028*
H123	0.1711	0.8516	0.8899	0.028*
C13	0.50570 (9)	0.86932 (9)	0.91338 (5)	0.02265 (18)
H131	0.5819	0.8120	0.9149	0.034*
H132	0.4979	0.9076	0.9621	0.034*
H133	0.5213	0.9323	0.8761	0.034*
C14	0.13430 (8)	0.58406 (7)	0.67361 (4)	0.01339 (14)
C15	0.01167 (9)	0.67043 (8)	0.67824 (5)	0.01810 (16)
H151	0.0321	0.7477	0.6538	0.027*
H152	−0.0073	0.6857	0.7303	0.027*
H153	−0.0677	0.6328	0.6536	0.027*
C16	0.10502 (9)	0.46117 (8)	0.71123 (5)	0.01891 (16)
H161	0.0281	0.4214	0.6854	0.028*
H162	0.0832	0.4753	0.7630	0.028*
H163	0.1851	0.4087	0.7091	0.028*
C17	0.15173 (9)	0.55772 (9)	0.59104 (5)	0.02034 (17)
H171	0.0679	0.5223	0.5699	0.031*
H172	0.2266	0.5002	0.5853	0.031*
H173	0.1718	0.6338	0.5652	0.031*

C18	0.88894 (9)	0.79959 (8)	0.48030 (5)	0.01788 (16)
H181	0.9319	0.7183	0.4773	0.021*
H182	0.9568	0.8574	0.5015	0.021*
C19	0.84370 (9)	0.84111 (8)	0.40378 (5)	0.01676 (16)
H191	0.7730	0.7845	0.3843	0.020*
H192	0.9217	0.8356	0.3709	0.020*
C20	0.78775 (10)	0.97033 (8)	0.40020 (5)	0.02082 (17)
H201	0.8581	1.0278	0.4191	0.025*
H202	0.7091	0.9765	0.4326	0.025*
C21	0.74391 (11)	1.00668 (9)	0.32151 (5)	0.0262 (2)
H211	0.8211	0.9992	0.2891	0.039*
H212	0.7119	1.0912	0.3213	0.039*
H213	0.6705	0.9530	0.3036	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0188 (3)	0.0195 (3)	0.0149 (3)	−0.0044 (2)	0.0074 (2)	−0.0049 (2)
O2	0.0176 (3)	0.0192 (3)	0.0221 (3)	−0.0039 (2)	0.0062 (2)	−0.0063 (2)
O3	0.0112 (3)	0.0167 (3)	0.0131 (3)	−0.0005 (2)	0.00417 (19)	0.0023 (2)
C1	0.0147 (3)	0.0142 (3)	0.0113 (3)	0.0013 (3)	0.0026 (3)	0.0003 (2)
C2	0.0140 (3)	0.0155 (3)	0.0147 (3)	0.0002 (3)	0.0051 (3)	0.0005 (3)
C3	0.0139 (4)	0.0168 (4)	0.0218 (4)	0.0016 (3)	0.0080 (3)	0.0037 (3)
C4	0.0118 (3)	0.0139 (3)	0.0163 (3)	0.0015 (3)	0.0045 (3)	0.0024 (3)
C5	0.0109 (3)	0.0144 (3)	0.0166 (3)	−0.0007 (3)	0.0011 (3)	0.0007 (3)
C6	0.0113 (3)	0.0119 (3)	0.0122 (3)	0.0006 (2)	0.0002 (2)	0.0006 (2)
C7	0.0095 (3)	0.0121 (3)	0.0115 (3)	0.0009 (2)	0.0023 (2)	0.0015 (2)
C8	0.0115 (3)	0.0117 (3)	0.0116 (3)	0.0010 (2)	0.0010 (2)	0.0010 (2)
C9	0.0148 (3)	0.0135 (3)	0.0120 (3)	0.0020 (3)	0.0032 (3)	0.0008 (3)
C10	0.0144 (3)	0.0139 (3)	0.0127 (3)	0.0004 (3)	−0.0003 (3)	−0.0009 (3)
C11	0.0297 (5)	0.0188 (4)	0.0122 (3)	0.0008 (3)	−0.0028 (3)	0.0010 (3)
C12	0.0209 (4)	0.0176 (4)	0.0169 (4)	0.0051 (3)	0.0011 (3)	−0.0027 (3)
C13	0.0197 (4)	0.0253 (4)	0.0227 (4)	−0.0043 (3)	−0.0025 (3)	−0.0080 (3)
C14	0.0124 (3)	0.0151 (3)	0.0126 (3)	0.0002 (3)	−0.0008 (3)	−0.0006 (3)
C15	0.0137 (4)	0.0215 (4)	0.0189 (4)	0.0034 (3)	−0.0025 (3)	−0.0002 (3)
C16	0.0194 (4)	0.0162 (4)	0.0209 (4)	−0.0042 (3)	−0.0033 (3)	−0.0003 (3)
C17	0.0198 (4)	0.0272 (4)	0.0139 (3)	0.0013 (3)	−0.0016 (3)	−0.0039 (3)
C18	0.0156 (4)	0.0222 (4)	0.0162 (4)	0.0013 (3)	0.0067 (3)	−0.0024 (3)
C19	0.0170 (4)	0.0184 (4)	0.0153 (3)	−0.0011 (3)	0.0059 (3)	−0.0031 (3)
C20	0.0236 (4)	0.0184 (4)	0.0206 (4)	0.0003 (3)	0.0028 (3)	−0.0029 (3)
C21	0.0306 (5)	0.0238 (4)	0.0242 (4)	0.0014 (4)	0.0018 (4)	0.0031 (4)

Geometric parameters (Å, º)

O1—C1	1.3330 (10)	C12—H122	0.9800
O1—C18	1.4606 (11)	C12—H123	0.9800
O2—C1	1.2130 (11)	C13—H131	0.9800
O3—C7	1.3840 (10)	C13—H132	0.9800

O3—H3	0.841 (13)	C13—H133	0.9800
C1—C2	1.5077 (12)	C14—C17	1.5347 (13)
C2—C3	1.5341 (13)	C14—C16	1.5418 (13)
C2—H21	0.9900	C14—C15	1.5419 (13)
C2—H22	0.9900	C15—H151	0.9800
C3—C4	1.5130 (12)	C15—H152	0.9800
C3—H31	0.9900	C15—H153	0.9800
C3—H32	0.9900	C16—H161	0.9800
C4—C9	1.3886 (12)	C16—H162	0.9800
C4—C5	1.3897 (12)	C16—H163	0.9800
C5—C6	1.3945 (12)	C17—H171	0.9800
C5—H51	0.9500	C17—H172	0.9800
C6—C7	1.4088 (11)	C17—H173	0.9800
C6—C10	1.5379 (12)	C18—C19	1.5090 (13)
C7—C8	1.4068 (11)	C18—H181	0.9900
C8—C9	1.3985 (12)	C18—H182	0.9900
C8—C14	1.5386 (12)	C19—C20	1.5223 (14)
C9—H91	0.9500	C19—H191	0.9900
C10—C13	1.5315 (13)	C19—H192	0.9900
C10—C11	1.5394 (13)	C20—C21	1.5253 (14)
C10—C12	1.5403 (13)	C20—H201	0.9900
C11—H111	0.9800	C20—H202	0.9900
C11—H112	0.9800	C21—H211	0.9800
C11—H113	0.9800	C21—H212	0.9800
C12—H121	0.9800	C21—H213	0.9800

C1—O1—C18	118.24 (7)	C10—C13—H132	109.5
C7—O3—H3	109.6 (8)	H131—C13—H132	109.5
O2—C1—O1	123.34 (8)	C10—C13—H133	109.5
O2—C1—C2	124.88 (7)	H131—C13—H133	109.5
O1—C1—C2	111.77 (7)	H132—C13—H133	109.5
C1—C2—C3	112.61 (7)	C17—C14—C8	111.72 (7)
C1—C2—H21	109.1	C17—C14—C16	107.01 (7)
C3—C2—H21	109.1	C8—C14—C16	110.51 (7)
C1—C2—H22	109.1	C17—C14—C15	106.39 (7)
C3—C2—H22	109.1	C8—C14—C15	110.34 (7)
H21—C2—H22	107.8	C16—C14—C15	110.77 (7)
C4—C3—C2	112.84 (7)	C14—C15—H151	109.5
C4—C3—H31	109.0	C14—C15—H152	109.5
C2—C3—H31	109.0	H151—C15—H152	109.5
C4—C3—H32	109.0	C14—C15—H153	109.5
C2—C3—H32	109.0	H151—C15—H153	109.5
H31—C3—H32	107.8	H152—C15—H153	109.5
C9—C4—C5	118.66 (7)	C14—C16—H161	109.5
C9—C4—C3	120.95 (8)	C14—C16—H162	109.5
C5—C4—C3	120.38 (8)	H161—C16—H162	109.5
C4—C5—C6	122.07 (7)	C14—C16—H163	109.5
C4—C5—H51	119.0	H161—C16—H163	109.5

C6—C5—H51	119.0	H162—C16—H163	109.5
C5—C6—C7	117.43 (7)	C14—C17—H171	109.5
C5—C6—C10	121.02 (7)	C14—C17—H172	109.5
C7—C6—C10	121.51 (7)	H171—C17—H172	109.5
O3—C7—C8	118.87 (7)	C14—C17—H173	109.5
O3—C7—C6	118.78 (7)	H171—C17—H173	109.5
C8—C7—C6	122.27 (7)	H172—C17—H173	109.5
C9—C8—C7	117.06 (7)	O1—C18—C19	109.95 (7)
C9—C8—C14	121.21 (7)	O1—C18—H181	109.7
C7—C8—C14	121.73 (7)	C19—C18—H181	109.7
C4—C9—C8	122.34 (8)	O1—C18—H182	109.7
C4—C9—H91	118.8	C19—C18—H182	109.7
C8—C9—H91	118.8	H181—C18—H182	108.2
C13—C10—C6	111.53 (7)	C18—C19—C20	114.58 (7)
C13—C10—C11	106.90 (7)	C18—C19—H191	108.6
C6—C10—C11	111.49 (7)	C20—C19—H191	108.6
C13—C10—C12	106.97 (8)	C18—C19—H192	108.6
C6—C10—C12	109.28 (7)	C20—C19—H192	108.6
C11—C10—C12	110.57 (7)	H191—C19—H192	107.6
C10—C11—H111	109.5	C19—C20—C21	111.99 (7)
C10—C11—H112	109.5	C19—C20—H201	109.2
H111—C11—H112	109.5	C21—C20—H201	109.2
C10—C11—H113	109.5	C19—C20—H202	109.2
H111—C11—H113	109.5	C21—C20—H202	109.2
H112—C11—H113	109.5	H201—C20—H202	107.9
C10—C12—H121	109.5	C20—C21—H211	109.5
C10—C12—H122	109.5	C20—C21—H212	109.5
H121—C12—H122	109.5	H211—C21—H212	109.5
C10—C12—H123	109.5	C20—C21—H213	109.5
H121—C12—H123	109.5	H211—C21—H213	109.5
H122—C12—H123	109.5	H212—C21—H213	109.5
C10—C13—H131	109.5		

C18—O1—C1—O2	−2.22 (12)	C5—C4—C9—C8	−2.71 (12)
C18—O1—C1—C2	177.72 (7)	C3—C4—C9—C8	178.29 (7)
O2—C1—C2—C3	−126.23 (9)	C7—C8—C9—C4	−0.01 (11)
O1—C1—C2—C3	53.83 (10)	C14—C8—C9—C4	179.18 (7)
C1—C2—C3—C4	178.11 (7)	C5—C6—C10—C13	0.63 (10)
C2—C3—C4—C9	100.16 (9)	C7—C6—C10—C13	−176.93 (7)
C2—C3—C4—C5	−78.82 (10)	C5—C6—C10—C11	−118.79 (8)
C9—C4—C5—C6	1.94 (12)	C7—C6—C10—C11	63.65 (10)
C3—C4—C5—C6	−179.05 (7)	C5—C6—C10—C12	118.69 (9)
C4—C5—C6—C7	1.47 (11)	C7—C6—C10—C12	−58.88 (10)
C4—C5—C6—C10	−176.19 (7)	C9—C8—C14—C17	−3.54 (10)
C5—C6—C7—O3	178.93 (7)	C7—C8—C14—C17	175.62 (7)
C10—C6—C7—O3	−3.42 (11)	C9—C8—C14—C16	115.49 (8)
C5—C6—C7—C8	−4.35 (11)	C7—C8—C14—C16	−65.36 (10)
C10—C6—C7—C8	173.29 (7)	C9—C8—C14—C15	−121.67 (8)

O3—C7—C8—C9	−179.65 (7)	C7—C8—C14—C15	57.49 (10)
C6—C7—C8—C9	3.64 (11)	C1—O1—C18—C19	−108.05 (9)
O3—C7—C8—C14	1.16 (11)	O1—C18—C19—C20	64.77 (9)
C6—C7—C8—C14	−175.55 (7)	C18—C19—C20—C21	180.00 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2^{i}	0.841 (13)	1.905 (13)	2.7399 (13)	172.1 (12)

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