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(*Z*)-3-(4-Methylbenzylidene)-4-oxopentanoic acid

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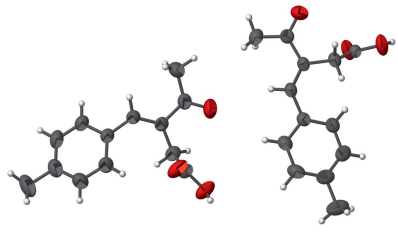
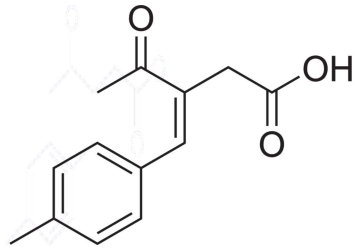
The title compound, $C_{13}H_{14}O_3$, a levulinic acid derivative, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The compound adopts a *Z* configuration about the C=C bonds in both molecules. The dihedral angle between the toluene ring and the carboxylic acid group is 72.83 (7)° in molecule *A* and 83.64 (8)° in molecule *B*. The toluene rings are inclined to the ketone substituents by 27.03 (9)° for *A* and 30.84 (6)° for *B*. In the crystal, like molecules are linked by pairs of O—H···O hydrogen bonds, forming *A*–*A* and *B*-*B* inversion dimers.

3D view



Chemical scheme



Structure description

Levulinic acid derivatives are known to possess a wide spectrum of pharmacological activities and are used in photodynamic therapy in gastroenterology (Mordon *et al.* 2005) and as drugs for prostate cancer (Colin *et al.* 2011). They are also reactants for the synthesis of other heterocyclic compounds such as pyridazinone derivatives (Boukharsa *et al.* 2015, 2016).

In this paper we report the crystal structure determination of the title compound, Fig. 1, which crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The dihedral angles between the toluene ring planes and the carboxylic acid groups O4/C14/O5/C15 and O1/O2/C1/C2/C3 are 72.83 (7)° in molecule A and 83.64 (8)° in molecule B. The toluene rings are inclined to the C16/C24/O6/C25 and C3/C11/O3/C12 ketone substituents by 27.03 (9)° for *A* and 30.84 (6)° for *B*.

In the title compound, the C—O [1.3056 (15) and 1.2981 (13) Å] and C=O [1.2132 (16) and 1.2201 (14) Å] bond distances agree well with the values given by Allen *et al.* (1987) for a variety of carboxylic acid groups (C—O 1.308 Å and C=O 1.214 Å). The bond angles at the central C atoms in the carboxylic acid groups [O1—C1—C2

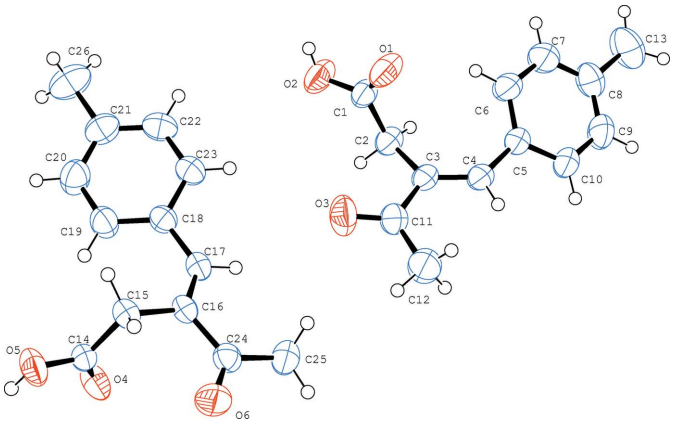


Figure 1
The asymmetric unit of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level.

123.22 (12), O2—C1—C2 113.64 (12)° and O4–C14–C15 122.88 (10) and O5–C14–C15 123.19 (10)°] are also similar to the mean values specified by Borthwick (1980) for a typical carboxylic acids [O2—C1—C2 123 (2)°, O1—C1—C2 112 (2)°].

In the crystal, molecules are linked by pairs of O2—H2···O1 and O5—H5···O4 hydrogen bonds (Table 1, Figs. 2 and 3), forming classical *A*–*A* and *B*–*B* carboxylic acid inversion dimers.

Synthesis and crystallization

An ice-cooled mixture of *o*-methylbenzaldehyde (0.02 mol) and levulinic acid (0.03 mol) was saturated with dry hydrogen chloride (HCl). Then, the mixture was stirred for 24 h at room temperature. The resulting precipitate was filtered off and washed with ethyl acetate. The crude product was crystallized

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O4^{i}	0.82	1.82	2.6310 (12)	171
O2—H2···O1^{ii}	0.82	1.85	2.6714 (15)	177

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{14}O_3$
M_r	218.25
Crystal system, space group	Monoclinic, $P2_1/a$
Temperature (K)	296
a, b, c (Å)	9.2491 (5), 18.1423 (10), 14.3719 (7)
β (°)	96.610 (3)
V (Å^3)	2395.6 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.3 × 0.2 × 0.15
Data collection	
Diffractometer	Bruker X8 *APEX*
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.91, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	129996, 7673, 5039
R_{int}	0.078
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.726
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.174, 1.05
No. of reflections	7673
No. of parameters	295
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.16

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

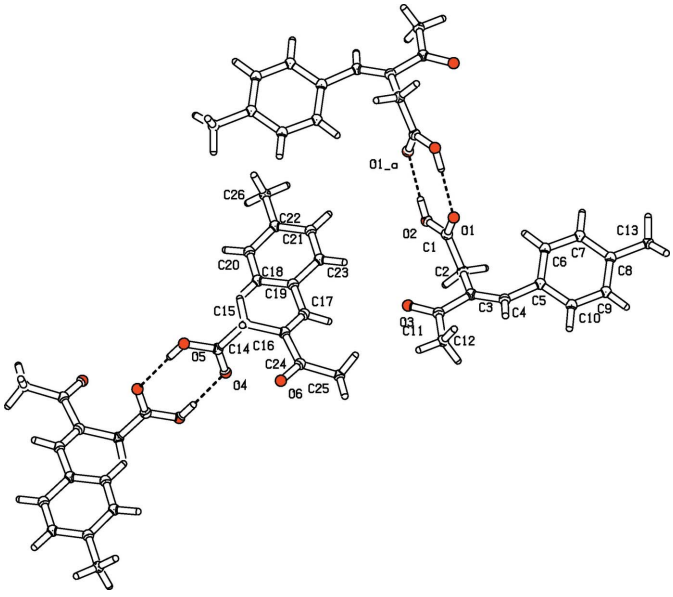


Figure 2
A view of the pairs of *A*–*A* and *B*–*B* inversion dimers formed by O—H···O hydrogen bonds.

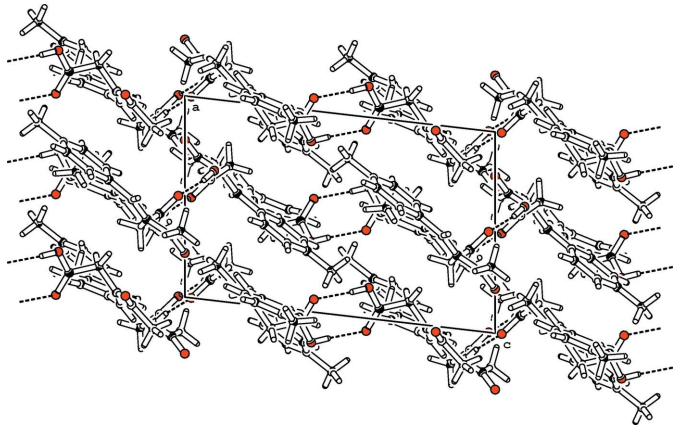


Figure 3
The three-dimensional structure in the unit cell, viewed along the *b* axis. Hydrogen-bonding interactions are shown as dashed lines.

from ethanol to afford colourless crystals (yield = 87%; m.p. = 144°C) (Boukharsa *et al.* 2016, El Marrakchi *et al.* 2014)].

Refinement

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

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full crystallographic data

IUCrData (2016). **1**, x162003 [https://doi.org/10.1107/S2414314616020034]

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Crystal data

$C_{13}H_{14}O_3$
M_r = 218.25
Monoclinic, $P2_1/a$
a = 9.2491 (5) Å
b = 18.1423 (10) Å
c = 14.3719 (7) Å
β = 96.610 (3)°
V = 2395.6 (2) Å^3
Z = 8
$F(000)$ = 928
D_x = 1.210 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7673 reflections
θ = 2.3–31.1°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.3 × 0.2 × 0.15 mm

Data collection

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.91, T_{max} = 0.98
129996 measured reflections
7673 independent reflections
5039 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 31.1°, θ_{min} = 2.3°
h = −13→13
k = −26→26
l = −18→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.174
S = 1.05
7673 reflections
295 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0946P)^2 + 0.1975P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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}
C16	0.13525 (12)	0.70579 (6)	0.12254 (8)	0.0392 (2)
C14	0.09904 (12)	0.57199 (6)	0.08109 (8)	0.0387 (2)
O4	−0.00001 (11)	0.58848 (5)	0.02117 (7)	0.0599 (3)
C17	0.04540 (12)	0.74580 (6)	0.16941 (8)	0.0416 (2)
H17	0.0348	0.7949	0.1511	0.050*
O5	0.14539 (12)	0.50486 (5)	0.09445 (7)	0.0624 (3)
H5	0.0926	0.4767	0.0613	0.094*
O6	0.28038 (12)	0.69915 (6)	0.00008 (8)	0.0663 (3)
C15	0.17930 (13)	0.62729 (6)	0.14503 (8)	0.0430 (2)
H15A	0.2828	0.6221	0.1412	0.052*
H15B	0.1622	0.6166	0.2090	0.052*
C18	−0.03845 (13)	0.72349 (6)	0.24511 (8)	0.0433 (3)
C24	0.20185 (13)	0.73769 (7)	0.04260 (8)	0.0453 (3)
C19	−0.09393 (16)	0.65281 (7)	0.25495 (11)	0.0574 (3)
H19	−0.0774	0.6166	0.2116	0.069*
C23	−0.07381 (15)	0.77700 (7)	0.30853 (9)	0.0518 (3)
H23	−0.0441	0.8255	0.3017	0.062*
C25	0.17203 (18)	0.81607 (8)	0.01331 (11)	0.0616 (4)
H25A	0.0695	0.8225	−0.0044	0.092*
H25B	0.2239	0.8276	−0.0390	0.092*
H25C	0.2036	0.8484	0.0646	0.092*
C22	−0.15266 (16)	0.75873 (9)	0.38157 (10)	0.0613 (4)
H22	−0.1735	0.7951	0.4236	0.074*
C21	−0.20095 (16)	0.68771 (9)	0.39341 (10)	0.0608 (3)
C20	−0.17302 (18)	0.63566 (9)	0.32788 (12)	0.0658 (4)
H20	−0.2082	0.5880	0.3329	0.079*
C26	−0.2846 (2)	0.66728 (13)	0.47373 (13)	0.0872 (6)
H26A	−0.2198	0.6452	0.5229	0.131*
H26B	−0.3600	0.6328	0.4524	0.131*
H26C	−0.3273	0.7108	0.4971	0.131*
C3	0.01570 (14)	1.08093 (7)	0.21990 (8)	0.0465 (3)
O1	0.06317 (11)	1.04595 (6)	0.41565 (7)	0.0700 (3)
O2	−0.15248 (12)	0.99179 (7)	0.40738 (8)	0.0734 (3)
H2	−0.1222	0.9794	0.4609	0.110*
C4	0.07038 (15)	1.14814 (7)	0.20654 (8)	0.0488 (3)
H4	0.1413	1.1498	0.1657	0.059*
C5	0.03529 (15)	1.21933 (7)	0.24653 (9)	0.0486 (3)
O3	0.02795 (14)	0.95429 (6)	0.19154 (10)	0.0786 (3)
C2	−0.10518 (14)	1.06384 (8)	0.27826 (9)	0.0521 (3)
H2A	−0.1592	1.1088	0.2865	0.063*
H2B	−0.1714	1.0291	0.2444	0.063*
C1	−0.05470 (14)	1.03229 (7)	0.37301 (9)	0.0498 (3)
C11	0.06928 (16)	1.01546 (7)	0.17210 (10)	0.0557 (3)
C10	0.04781 (18)	1.28227 (8)	0.19252 (11)	0.0628 (4)
H10	0.0781	1.2780	0.1333	0.075*

C9	0.0157 (2)	1.35095 (8)	0.22602 (13)	0.0708 (4)
H9	0.0228	1.3920	0.1880	0.085*
C6	−0.0045 (2)	1.22914 (8)	0.33599 (10)	0.0686 (4)
H6	−0.0104	1.1885	0.3748	0.082*
C8	−0.02629 (17)	1.36043 (8)	0.31340 (13)	0.0656 (4)
C7	−0.0355 (2)	1.29855 (9)	0.36803 (13)	0.0755 (5)
H7	−0.0632	1.3036	0.4279	0.091*
C12	0.1763 (2)	1.02402 (9)	0.10182 (14)	0.0850 (6)
H12A	0.2635	1.0468	0.1313	0.128*
H12B	0.1345	1.0543	0.0509	0.128*
H12C	0.1992	0.9764	0.0783	0.128*
C13	−0.0593 (3)	1.43579 (10)	0.35049 (19)	0.0979 (7)
H13A	−0.1600	1.4474	0.3327	0.147*
H13B	0.0007	1.4719	0.3248	0.147*
H13C	−0.0396	1.4359	0.4175	0.147*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C16	0.0393 (5)	0.0342 (5)	0.0431 (5)	−0.0027 (4)	0.0007 (4)	−0.0051 (4)
C14	0.0429 (5)	0.0330 (5)	0.0408 (5)	0.0002 (4)	0.0072 (4)	−0.0007 (4)
O4	0.0634 (6)	0.0388 (4)	0.0713 (6)	0.0057 (4)	−0.0183 (5)	−0.0112 (4)
C17	0.0439 (6)	0.0341 (5)	0.0462 (6)	−0.0009 (4)	0.0019 (4)	−0.0032 (4)
O5	0.0852 (7)	0.0319 (4)	0.0637 (6)	0.0025 (4)	−0.0193 (5)	−0.0019 (4)
O6	0.0717 (7)	0.0660 (6)	0.0657 (6)	0.0078 (5)	0.0266 (5)	−0.0053 (5)
C15	0.0436 (6)	0.0361 (5)	0.0482 (6)	0.0011 (4)	0.0008 (5)	−0.0045 (4)
C18	0.0423 (6)	0.0419 (6)	0.0455 (6)	0.0032 (4)	0.0044 (5)	−0.0032 (4)
C24	0.0433 (6)	0.0447 (6)	0.0480 (6)	−0.0051 (5)	0.0054 (5)	−0.0051 (5)
C19	0.0628 (8)	0.0451 (7)	0.0677 (8)	−0.0040 (6)	0.0215 (7)	−0.0079 (6)
C23	0.0554 (7)	0.0469 (6)	0.0534 (7)	0.0041 (5)	0.0078 (6)	−0.0071 (5)
C25	0.0718 (9)	0.0494 (7)	0.0654 (8)	−0.0062 (6)	0.0157 (7)	0.0081 (6)
C22	0.0626 (8)	0.0692 (9)	0.0538 (7)	0.0071 (7)	0.0138 (6)	−0.0123 (6)
C21	0.0527 (7)	0.0751 (9)	0.0561 (8)	0.0068 (7)	0.0134 (6)	0.0073 (7)
C20	0.0665 (9)	0.0574 (8)	0.0772 (10)	−0.0043 (7)	0.0237 (8)	0.0057 (7)
C26	0.0783 (11)	0.1172 (16)	0.0709 (11)	0.0043 (11)	0.0297 (9)	0.0171 (10)
C3	0.0565 (7)	0.0444 (6)	0.0386 (5)	0.0011 (5)	0.0052 (5)	0.0067 (4)
O1	0.0603 (6)	0.0935 (8)	0.0553 (5)	−0.0173 (5)	0.0034 (5)	0.0272 (5)
O2	0.0680 (7)	0.0907 (8)	0.0612 (6)	−0.0252 (6)	0.0072 (5)	0.0242 (6)
C4	0.0609 (7)	0.0447 (6)	0.0422 (6)	0.0004 (5)	0.0117 (5)	0.0032 (5)
C5	0.0566 (7)	0.0441 (6)	0.0461 (6)	−0.0024 (5)	0.0096 (5)	0.0031 (5)
O3	0.0910 (8)	0.0423 (5)	0.1056 (9)	−0.0033 (5)	0.0243 (7)	0.0054 (5)
C2	0.0519 (7)	0.0565 (7)	0.0480 (6)	−0.0022 (6)	0.0054 (5)	0.0083 (5)
C1	0.0531 (7)	0.0497 (6)	0.0478 (6)	−0.0048 (5)	0.0116 (5)	0.0078 (5)
C11	0.0659 (8)	0.0439 (6)	0.0575 (7)	0.0017 (6)	0.0082 (6)	0.0034 (5)
C10	0.0833 (10)	0.0482 (7)	0.0602 (8)	−0.0094 (7)	0.0223 (7)	0.0059 (6)
C9	0.0897 (11)	0.0441 (7)	0.0804 (10)	−0.0052 (7)	0.0169 (9)	0.0099 (7)
C6	0.1076 (13)	0.0497 (7)	0.0519 (8)	0.0014 (7)	0.0235 (8)	0.0034 (6)
C8	0.0626 (9)	0.0484 (7)	0.0857 (10)	0.0020 (6)	0.0081 (8)	−0.0074 (7)

C7	0.1064 (14)	0.0575 (9)	0.0670 (9)	0.0010 (8)	0.0295 (9)	−0.0100 (7)
C12	0.1175 (15)	0.0563 (9)	0.0903 (12)	0.0036 (9)	0.0507 (11)	−0.0076 (8)
C13	0.1082 (15)	0.0555 (9)	0.1306 (18)	0.0096 (10)	0.0164 (13)	−0.0239 (10)

Geometric parameters (Å, º)

C16—C17	1.3417 (16)	C3—C4	1.3424 (17)
C16—C15	1.5061 (15)	C3—C2	1.5052 (18)
C16—C24	1.4823 (17)	C3—C11	1.4854 (18)
C14—O4	1.2201 (14)	O1—C1	1.2132 (16)
C14—O5	1.2981 (13)	O2—H2	0.8200
C14—C15	1.4984 (15)	O2—C1	1.3056 (15)
C17—H17	0.9300	C4—H4	0.9300
C17—C18	1.4639 (17)	C4—C5	1.4651 (17)
O5—H5	0.8200	C5—C10	1.3931 (18)
O6—C24	1.2215 (15)	C5—C6	1.3890 (19)
C15—H15A	0.9700	O3—C11	1.2166 (16)
C15—H15B	0.9700	C2—H2A	0.9700
C18—C19	1.3943 (17)	C2—H2B	0.9700
C18—C23	1.3960 (17)	C2—C1	1.5012 (18)
C24—C25	1.4995 (18)	C11—C12	1.501 (2)
C19—H19	0.9300	C10—H10	0.9300
C19—C20	1.381 (2)	C10—C9	1.380 (2)
C23—H23	0.9300	C9—H9	0.9300
C23—C22	1.386 (2)	C9—C8	1.367 (2)
C25—H25A	0.9600	C6—H6	0.9300
C25—H25B	0.9600	C6—C7	1.382 (2)
C25—H25C	0.9600	C8—C7	1.378 (2)
C22—H22	0.9300	C8—C13	1.511 (2)
C22—C21	1.381 (2)	C7—H7	0.9300
C21—C20	1.379 (2)	C12—H12A	0.9600
C21—C26	1.508 (2)	C12—H12B	0.9600
C20—H20	0.9300	C12—H12C	0.9600
C26—H26A	0.9600	C13—H13A	0.9600
C26—H26B	0.9600	C13—H13B	0.9600
C26—H26C	0.9600	C13—H13C	0.9600
C17—C16—C15	124.87 (11)	C4—C3—C2	125.67 (12)
C17—C16—C24	120.97 (10)	C4—C3—C11	120.59 (12)
C24—C16—C15	114.16 (10)	C11—C3—C2	113.69 (11)
O4—C14—O5	122.88 (10)	C1—O2—H2	109.5
O4—C14—C15	123.19 (10)	C3—C4—H4	115.1
O5—C14—C15	113.93 (10)	C3—C4—C5	129.83 (12)
C16—C17—H17	115.3	C5—C4—H4	115.1
C16—C17—C18	129.44 (11)	C10—C5—C4	117.89 (12)
C18—C17—H17	115.3	C6—C5—C4	124.78 (11)
C14—O5—H5	109.5	C6—C5—C10	117.29 (13)
C16—C15—H15A	108.9	C3—C2—H2A	108.7

C16—C15—H15B	108.9	C3—C2—H2B	108.7
C14—C15—C16	113.50 (9)	H2A—C2—H2B	107.6
C14—C15—H15A	108.9	C1—C2—C3	114.24 (11)
C14—C15—H15B	108.9	C1—C2—H2A	108.7
H15A—C15—H15B	107.7	C1—C2—H2B	108.7
C19—C18—C17	124.22 (11)	O1—C1—O2	123.04 (12)
C19—C18—C23	117.17 (12)	O1—C1—C2	123.22 (11)
C23—C18—C17	118.48 (11)	O2—C1—C2	113.64 (12)
C16—C24—C25	120.56 (11)	C3—C11—C12	120.61 (12)
O6—C24—C16	119.23 (11)	O3—C11—C3	119.53 (13)
O6—C24—C25	120.20 (12)	O3—C11—C12	119.85 (13)
C18—C19—H19	119.4	C5—C10—H10	119.6
C20—C19—C18	121.16 (13)	C9—C10—C5	120.71 (14)
C20—C19—H19	119.4	C9—C10—H10	119.6
C18—C23—H23	119.6	C10—C9—H9	119.0
C22—C23—C18	120.77 (13)	C8—C9—C10	121.94 (14)
C22—C23—H23	119.6	C8—C9—H9	119.0
C24—C25—H25A	109.5	C5—C6—H6	119.6
C24—C25—H25B	109.5	C7—C6—C5	120.82 (14)
C24—C25—H25C	109.5	C7—C6—H6	119.6
H25A—C25—H25B	109.5	C9—C8—C7	117.62 (14)
H25A—C25—H25C	109.5	C9—C8—C13	121.87 (16)
H25B—C25—H25C	109.5	C7—C8—C13	120.51 (17)
C23—C22—H22	119.2	C6—C7—H7	119.2
C21—C22—C23	121.50 (13)	C8—C7—C6	121.57 (15)
C21—C22—H22	119.2	C8—C7—H7	119.2
C22—C21—C26	121.71 (16)	C11—C12—H12A	109.5
C20—C21—C22	117.79 (13)	C11—C12—H12B	109.5
C20—C21—C26	120.49 (16)	C11—C12—H12C	109.5
C19—C20—H20	119.3	H12A—C12—H12B	109.5
C21—C20—C19	121.42 (14)	H12A—C12—H12C	109.5
C21—C20—H20	119.3	H12B—C12—H12C	109.5
C21—C26—H26A	109.5	C8—C13—H13A	109.5
C21—C26—H26B	109.5	C8—C13—H13B	109.5
C21—C26—H26C	109.5	C8—C13—H13C	109.5
H26A—C26—H26B	109.5	H13A—C13—H13B	109.5
H26A—C26—H26C	109.5	H13A—C13—H13C	109.5
H26B—C26—H26C	109.5	H13B—C13—H13C	109.5

C16—C17—C18—C19	−31.0 (2)	C3—C4—C5—C10	−148.97 (15)
C16—C17—C18—C23	153.27 (13)	C3—C4—C5—C6	33.5 (2)
O4—C14—C15—C16	−5.22 (17)	C3—C2—C1—O1	28.9 (2)
C17—C16—C15—C14	101.54 (13)	C3—C2—C1—O2	−154.42 (12)
C17—C16—C24—O6	−178.25 (12)	C4—C3—C2—C1	−101.98 (15)
C17—C16—C24—C25	1.01 (17)	C4—C3—C11—O3	173.44 (14)
C17—C18—C19—C20	−179.59 (14)	C4—C3—C11—C12	−5.2 (2)
C17—C18—C23—C22	−179.83 (12)	C4—C5—C10—C9	179.70 (15)
O5—C14—C15—C16	174.08 (10)	C4—C5—C6—C7	179.85 (16)

C15—C16—C17—C18	−5.48 (19)	C5—C10—C9—C8	1.4 (3)
C15—C16—C24—O6	2.48 (16)	C5—C6—C7—C8	−0.9 (3)
C15—C16—C24—C25	−178.26 (11)	C2—C3—C4—C5	3.4 (2)
C18—C19—C20—C21	0.4 (2)	C2—C3—C11—O3	−9.04 (19)
C18—C23—C22—C21	−1.1 (2)	C2—C3—C11—C12	172.34 (15)
C24—C16—C17—C18	175.34 (11)	C11—C3—C4—C5	−179.38 (13)
C24—C16—C15—C14	−79.23 (12)	C11—C3—C2—C1	80.64 (15)
C19—C18—C23—C22	4.2 (2)	C10—C5—C6—C7	2.4 (3)
C23—C18—C19—C20	−3.8 (2)	C10—C9—C8—C7	0.2 (3)
C23—C22—C21—C20	−2.4 (2)	C10—C9—C8—C13	179.10 (18)
C23—C22—C21—C26	178.96 (15)	C9—C8—C7—C6	−0.4 (3)
C22—C21—C20—C19	2.8 (2)	C6—C5—C10—C9	−2.6 (2)
C26—C21—C20—C19	−178.59 (16)	C13—C8—C7—C6	−179.39 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O4^{i}	0.82	1.82	2.6310 (12)	171
O2—H2···O1^{ii}	0.82	1.85	2.6714 (15)	177

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