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1-Hydroxycyclopentane-1-carboxylic acid

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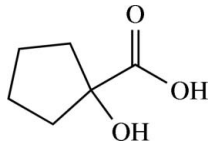
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.050; wR factor = 0.144; data-to-parameter ratio = 15.4.

The title compound, $C_6H_{10}O_3$, crystallizes with three independent molecules in the asymmetric unit. In all three molecules, which have similar envelope conformations, the cyclopentane ring is arranged skew to the carboxyl group. Intermolecular O—H···O hydrogen bonds link the molecules into two-dimensional layers parallel to the *ab* plane.

Related literature

The title compound was prepared according to a standard procedure (Becker *et al.*, 2001).



Experimental

Crystal data

$C_6H_{10}O_3$
M_r = 130.14
Monoclinic, $P2_1/c$
a = 16.0000 (16) Å
b = 6.3490 (4) Å
c = 19.664 (2) Å
β = 96.812 (12)°
V = 1983.4 (3) Å^3
Z = 12
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 200 (2) K
0.50 × 0.20 × 0.11 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1997)
T_{min} = 0.977, T_{max} = 0.989
13242 measured reflections
3774 independent reflections
2574 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
S = 0.95
3774 reflections
245 parameters
Only H-atom displacement parameters refined
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O12—H12···O22^{i}	0.84	1.86	2.684 (2)	165
O111—H111···O112^{ii}	0.84	1.80	2.624 (2)	167
O22—H22···O32^{iii}	0.84	1.93	2.757 (2)	169
O211—H211···O212^{iv}	0.84	1.82	2.6559 (19)	177
O32—H32···O12^{v}	0.84	1.89	2.710 (2)	166
O311—H311···O312^{vi}	0.84	1.79	2.629 (2)	175

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

Data collection: *IPDS Software* (Stoe & Cie, 1996); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2295).

References

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supplementary materials

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1-Hydroxycyclopentane-1-carboxylic acid

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Comment

The title compound, $C_6H_{10}O_3$, was prepared as chelating molecule bearing the conformationally flexible cyclopentane group. It was obtained upon acidic hydrolysis of the cyanohydrin of cyclopentanone. The cyclopentane ring adopts a skew orientation to the planar carboxyl group. Hydrophobic and hydrophilic sheets alternate along [001] (Figure 2). Each individual hydrophilic sheet is composed of the typical bidentately linked carboxylic-acid dimers. The dimer packing is supported by three symmetrically independent, laterally running, cooperative, linearly infinite hydrogen-bond systems which are exclusively formed by hydroxyl-OH vectors.

The molecular structure (Fig. 1) shows a carboxy- and a hydroxy-group attached to the cyclopentane ring.

The molecular packing (Fig. 2) shows O—H···O intermolecular hydrogen bonds (Table 2).

Experimental

The title compound was prepared according to standard procedures (Becker *et al.*, 2001) upon acidic hydrolysis of the cyanohydrin of cyclopentanone. Crystals suitable for X-ray analysis were directly obtained from the crystallized reaction product.

Refinement

All H atoms were located in a difference map and refined as riding on their parent atoms, with C—H = 0.99 Å and O—H = 0.84 Å. One common isotropic displacement parameter for all H atoms was refined to U_{iso}(H) = 0.0748 (17).

Figures

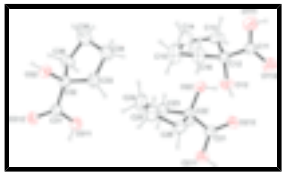

Fig. 1. Three independent molecules in asymmetric unit of (I), with atom labels and displacement ellipsoids drawn at the 50% probability level.

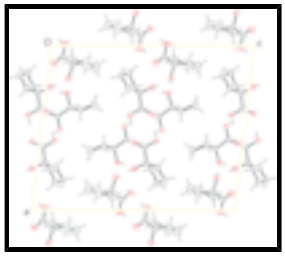

Fig. 2. The packing of (I), viewed along [0 1 0].

1-Hydroxycyclopentane-1-carboxylic acid

Crystal data

$C_6H_{10}O_3$	F_{000} = 840
M_r = 130.14	D_x = 1.307 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5000 reflections
a = 16.0000 (16) Å	θ = 2.3–25.9º
b = 6.3490 (4) Å	μ = 0.11 mm^{-1}
c = 19.664 (2) Å	T = 200 (2) K
β = 96.812 (12)º	Rod, colourless
V = 1983.4 (3) Å^3	0.50 × 0.20 × 0.11 mm
Z = 12	

Data collection

Stoe IPDS diffractometer	3774 independent reflections
Radiation source: fine-focus sealed tube	2574 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 200(2) K	θ_{max} = 25.9º
area detection scans	θ_{min} = 2.3º
Absorption correction: numerical (X-RED; Stoe & Cie, 1997)	h = −19→19
T_{min} = 0.977, T_{max} = 0.989	k = −7→7
13242 measured reflections	l = −24→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.050	Only H-atom displacement parameters refined
$wR(F^2)$ = 0.144	$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.95	$(\Delta/\sigma)_{max} < 0.001$
3774 reflections	$\Delta\rho_{max}$ = 0.61 e Å^{-3}
245 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\mathrm{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O12	0.19965 (8)	0.6718 (2)	0.10560 (7)	0.0364 (3)
H12	0.2196	0.7943	0.1064	0.0748 (17)*
O111	−0.01397 (10)	0.8320 (4)	0.06625 (10)	0.0740 (7)
H111	−0.0353	0.9189	0.0370	0.0748 (17)*
O112	0.10236 (10)	0.9290 (3)	0.02446 (9)	0.0517 (5)
C11	0.06518 (12)	0.8249 (4)	0.06479 (10)	0.0359 (5)
C12	0.11415 (11)	0.6807 (3)	0.11629 (10)	0.0332 (4)
C13	0.08053 (14)	0.4546 (4)	0.11271 (12)	0.0432 (5)
H131	0.0185	0.4533	0.1023	0.0748 (17)*
H132	0.1052	0.3731	0.0771	0.0748 (17)*
C14	0.1072 (2)	0.3651 (5)	0.18264 (16)	0.0776 (9)
H141	0.1581	0.2768	0.1819	0.0748 (17)*
H142	0.0618	0.2766	0.1975	0.0748 (17)*
C15	0.1257 (2)	0.5482 (5)	0.23127 (13)	0.0666 (8)
H151	0.0909	0.5387	0.2695	0.0748 (17)*
H152	0.1858	0.5481	0.2504	0.0748 (17)*
C16	0.10471 (16)	0.7461 (4)	0.19014 (11)	0.0460 (6)
H161	0.1442	0.8613	0.2055	0.0748 (17)*
H162	0.0465	0.7930	0.1943	0.0748 (17)*
O22	0.28938 (8)	0.0287 (2)	0.10435 (7)	0.0333 (3)
H22	0.2801	0.1239	0.0748	0.0748 (17)*
O211	0.51060 (9)	0.0212 (3)	0.09287 (7)	0.0465 (4)
H211	0.5374	0.0122	0.0588	0.0748 (17)*
O212	0.40014 (9)	−0.0017 (2)	0.01254 (7)	0.0375 (4)
C21	0.42968 (12)	0.0148 (3)	0.07252 (10)	0.0324 (4)
C22	0.37585 (12)	0.0299 (4)	0.13065 (10)	0.0336 (5)
C23	0.39049 (14)	−0.1550 (5)	0.18061 (11)	0.0476 (6)
H231	0.3581	−0.2802	0.1628	0.0748 (17)*
H232	0.4509	−0.1924	0.1884	0.0748 (17)*
C24	0.36000 (19)	−0.0771 (6)	0.24609 (13)	0.0733 (10)
H241	0.3964	−0.1317	0.2864	0.0748 (17)*
H242	0.3016	−0.1247	0.2489	0.0748 (17)*
C25	0.36404 (18)	0.1663 (6)	0.24395 (12)	0.0648 (8)
H251	0.3075	0.2276	0.2461	0.0748 (17)*
H252	0.4027	0.2204	0.2831	0.0748 (17)*
C26	0.39636 (15)	0.2230 (4)	0.17639 (11)	0.0490 (6)
H261	0.4578	0.2496	0.1832	0.0748 (17)*
H262	0.3675	0.3499	0.1560	0.0748 (17)*

O32	0.25059 (8)	0.1270 (2)	0.52112 (6)	0.0329 (3)
H32	0.2406	0.0209	0.5444	0.0748 (17)*
O311	0.42291 (9)	0.0291 (3)	0.42673 (7)	0.0458 (4)
H311	0.4743	0.0110	0.4399	0.0748 (17)*
O312	0.41433 (9)	0.0178 (3)	0.53879 (7)	0.0384 (4)
C31	0.38133 (12)	0.0366 (3)	0.47965 (9)	0.0308 (4)
C32	0.28721 (12)	0.0615 (3)	0.46198 (9)	0.0312 (4)
C33	0.26007 (14)	0.2220 (4)	0.40524 (11)	0.0426 (5)
H331	0.2452	0.3581	0.4252	0.0748 (17)*
H332	0.3060	0.2460	0.3765	0.0748 (17)*
C34	0.18311 (15)	0.1247 (5)	0.36266 (12)	0.0547 (7)
H341	0.1346	0.2222	0.3602	0.0748 (17)*
H342	0.1957	0.0947	0.3155	0.0748 (17)*
C35	0.16372 (14)	−0.0772 (4)	0.39858 (12)	0.0507 (6)
H351	0.1399	−0.1846	0.3653	0.0748 (17)*
H352	0.1235	−0.0516	0.4322	0.0748 (17)*
C36	0.24874 (12)	−0.1463 (4)	0.43407 (11)	0.0389 (5)
H361	0.2834	−0.2118	0.4013	0.0748 (17)*
H362	0.2423	−0.2470	0.4715	0.0748 (17)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O12	0.0293 (7)	0.0307 (8)	0.0486 (8)	−0.0011 (6)	0.0031 (6)	0.0015 (6)
O111	0.0356 (9)	0.0997 (17)	0.0874 (13)	0.0133 (10)	0.0095 (8)	0.0552 (13)
O112	0.0425 (9)	0.0562 (12)	0.0573 (10)	0.0042 (7)	0.0098 (7)	0.0238 (8)
C11	0.0309 (10)	0.0389 (13)	0.0388 (10)	0.0004 (8)	0.0073 (8)	0.0037 (9)
C12	0.0288 (10)	0.0323 (12)	0.0385 (10)	0.0000 (8)	0.0035 (7)	0.0016 (8)
C13	0.0361 (11)	0.0382 (14)	0.0557 (13)	−0.0067 (9)	0.0068 (9)	0.0002 (10)
C14	0.117 (3)	0.045 (2)	0.0694 (18)	−0.0041 (17)	0.0041 (17)	0.0184 (14)
C15	0.095 (2)	0.0574 (19)	0.0457 (14)	0.0041 (15)	0.0031 (14)	0.0116 (12)
C16	0.0596 (14)	0.0399 (15)	0.0392 (11)	0.0095 (10)	0.0088 (10)	−0.0002 (9)
O22	0.0282 (7)	0.0375 (9)	0.0346 (7)	−0.0020 (6)	0.0051 (5)	0.0076 (6)
O211	0.0289 (7)	0.0804 (13)	0.0303 (7)	−0.0023 (7)	0.0040 (6)	−0.0044 (7)
O212	0.0334 (7)	0.0513 (10)	0.0278 (7)	−0.0028 (6)	0.0036 (5)	−0.0039 (6)
C21	0.0308 (10)	0.0356 (13)	0.0308 (10)	−0.0026 (8)	0.0035 (7)	−0.0010 (8)
C22	0.0290 (9)	0.0425 (13)	0.0296 (10)	−0.0044 (8)	0.0055 (7)	0.0016 (8)
C23	0.0362 (11)	0.0629 (17)	0.0433 (12)	0.0046 (10)	0.0024 (9)	0.0192 (11)
C24	0.0648 (18)	0.115 (3)	0.0420 (14)	0.0050 (17)	0.0132 (12)	0.0246 (16)
C25	0.0625 (16)	0.100 (3)	0.0338 (12)	−0.0154 (16)	0.0128 (11)	−0.0114 (13)
C26	0.0454 (12)	0.0672 (18)	0.0369 (11)	−0.0174 (11)	0.0151 (9)	−0.0174 (11)
O32	0.0333 (7)	0.0326 (9)	0.0342 (7)	0.0020 (6)	0.0097 (5)	−0.0040 (6)
O311	0.0302 (7)	0.0780 (13)	0.0298 (7)	0.0093 (7)	0.0059 (6)	−0.0010 (7)
O312	0.0327 (7)	0.0554 (11)	0.0269 (7)	0.0057 (6)	0.0023 (5)	0.0020 (6)
C31	0.0311 (10)	0.0333 (12)	0.0283 (9)	0.0035 (8)	0.0045 (7)	−0.0013 (8)
C32	0.0309 (10)	0.0351 (12)	0.0281 (9)	0.0046 (8)	0.0056 (7)	−0.0024 (8)
C33	0.0421 (12)	0.0496 (15)	0.0360 (10)	0.0099 (10)	0.0048 (8)	0.0074 (10)
C34	0.0391 (12)	0.084 (2)	0.0391 (12)	0.0119 (12)	−0.0014 (9)	0.0080 (12)

C35	0.0365 (11)	0.0659 (18)	0.0474 (13)	0.0004 (11)	−0.0045 (9)	−0.0123 (12)
C36	0.0355 (11)	0.0415 (14)	0.0392 (11)	0.0023 (9)	0.0017 (8)	−0.0112 (9)

Geometric parameters (Å, °)

O12—C12	1.410 (2)	C23—H232	0.9900
O12—H12	0.8400	C24—C25	1.547 (5)
O111—C11	1.271 (3)	C24—H241	0.9900
O111—H111	0.8400	C24—H242	0.9900
O112—C11	1.238 (3)	C25—C26	1.525 (3)
C11—C12	1.513 (3)	C25—H251	0.9900
C12—C13	1.532 (3)	C25—H252	0.9900
C12—C16	1.535 (3)	C26—H261	0.9900
C13—C14	1.503 (4)	C26—H262	0.9900
C13—H131	0.9900	O32—C32	1.425 (2)
C13—H132	0.9900	O32—H32	0.8400
C14—C15	1.512 (4)	O311—C31	1.301 (2)
C14—H141	0.9900	O311—H311	0.8400
C14—H142	0.9900	O312—C31	1.225 (2)
C15—C16	1.510 (4)	C31—C32	1.513 (3)
C15—H151	0.9900	C32—C36	1.530 (3)
C15—H152	0.9900	C32—C33	1.535 (3)
C16—H161	0.9900	C33—C34	1.534 (3)
C16—H162	0.9900	C33—H331	0.9900
O22—C22	1.418 (2)	C33—H332	0.9900
O22—H22	0.8400	C34—C35	1.513 (4)
O211—C21	1.310 (2)	C34—H341	0.9900
O211—H211	0.8399	C34—H342	0.9900
O212—C21	1.222 (2)	C35—C36	1.518 (3)
C21—C22	1.514 (3)	C35—H351	0.9900
C22—C23	1.531 (3)	C35—H352	0.9900
C22—C26	1.533 (3)	C36—H361	0.9900
C23—C24	1.513 (4)	C36—H362	0.9900
C23—H231	0.9900		
C12—O12—H12	109.5	C23—C24—H241	110.4
C11—O111—H111	109.5	C25—C24—H241	110.4
O112—C11—O111	123.5 (2)	C23—C24—H242	110.4
O112—C11—C12	120.12 (18)	C25—C24—H242	110.4
O111—C11—C12	116.39 (18)	H241—C24—H242	108.6
O12—C12—C11	111.05 (16)	C26—C25—C24	106.2 (2)
O12—C12—C13	107.29 (17)	C26—C25—H251	110.5
C11—C12—C13	112.65 (17)	C24—C25—H251	110.5
O12—C12—C16	110.98 (17)	C26—C25—H252	110.5
C11—C12—C16	111.61 (17)	C24—C25—H252	110.5
C13—C12—C16	102.92 (18)	H251—C25—H252	108.7
C14—C13—C12	104.6 (2)	C25—C26—C22	104.6 (2)
C14—C13—H131	110.8	C25—C26—H261	110.8
C12—C13—H131	110.8	C22—C26—H261	110.8
C14—C13—H132	110.8	C25—C26—H262	110.8

C12—C13—H132	110.8	C22—C26—H262	110.8
H131—C13—H132	108.9	H261—C26—H262	108.9
C13—C14—C15	107.5 (2)	C32—O32—H32	109.5
C13—C14—H141	110.2	C31—O311—H311	109.5
C15—C14—H141	110.2	O312—C31—O311	123.52 (17)
C13—C14—H142	110.2	O312—C31—C32	122.24 (17)
C15—C14—H142	110.2	O311—C31—C32	114.19 (16)
H141—C14—H142	108.5	O32—C32—C31	109.73 (14)
C16—C15—C14	106.7 (2)	O32—C32—C36	110.95 (16)
C16—C15—H151	110.4	C31—C32—C36	109.85 (16)
C14—C15—H151	110.4	O32—C32—C33	106.93 (16)
C16—C15—H152	110.4	C31—C32—C33	115.09 (17)
C14—C15—H152	110.4	C36—C32—C33	104.16 (16)
H151—C15—H152	108.6	C34—C33—C32	105.6 (2)
C15—C16—C12	104.0 (2)	C34—C33—H331	110.6
C15—C16—H161	111.0	C32—C33—H331	110.6
C12—C16—H161	111.0	C34—C33—H332	110.6
C15—C16—H162	111.0	C32—C33—H332	110.6
C12—C16—H162	111.0	H331—C33—H332	108.8
H161—C16—H162	109.0	C35—C34—C33	106.38 (18)
C22—O22—H22	109.5	C35—C34—H341	110.5
C21—O211—H211	109.5	C33—C34—H341	110.5
O212—C21—O211	123.56 (18)	C35—C34—H342	110.5
O212—C21—C22	123.01 (17)	C33—C34—H342	110.5
O211—C21—C22	113.43 (16)	H341—C34—H342	108.6
O22—C22—C21	110.00 (15)	C34—C35—C36	103.73 (19)
O22—C22—C23	107.33 (16)	C34—C35—H351	111.0
C21—C22—C23	112.24 (18)	C36—C35—H351	111.0
O22—C22—C26	110.50 (18)	C34—C35—H352	111.0
C21—C22—C26	113.11 (17)	C36—C35—H352	111.0
C23—C22—C26	103.35 (18)	H351—C35—H352	109.0
C24—C23—C22	104.8 (2)	C35—C36—C32	102.47 (18)
C24—C23—H231	110.8	C35—C36—H361	111.3
C22—C23—H231	110.8	C32—C36—H361	111.3
C24—C23—H232	110.8	C35—C36—H362	111.3
C22—C23—H232	110.8	C32—C36—H362	111.3
H231—C23—H232	108.9	H361—C36—H362	109.2
C23—C24—C25	106.5 (2)		
O112—C11—C12—O12	−5.7 (3)	C26—C22—C23—C24	37.0 (2)
O111—C11—C12—O12	174.7 (2)	C22—C23—C24—C25	−23.2 (3)
O112—C11—C12—C13	−126.1 (2)	C23—C24—C25—C26	0.5 (3)
O111—C11—C12—C13	54.3 (3)	C24—C25—C26—C22	22.4 (3)
O112—C11—C12—C16	118.7 (2)	O22—C22—C26—C25	78.0 (2)
O111—C11—C12—C16	−60.9 (3)	C21—C22—C26—C25	−158.19 (19)
O12—C12—C13—C14	82.0 (2)	C23—C22—C26—C25	−36.6 (2)
C11—C12—C13—C14	−155.5 (2)	O312—C31—C32—O32	18.8 (3)
C16—C12—C13—C14	−35.2 (2)	O311—C31—C32—O32	−163.73 (18)
C12—C13—C14—C15	20.0 (3)	O312—C31—C32—C36	−103.4 (2)
C13—C14—C15—C16	3.3 (4)	O311—C31—C32—C36	74.0 (2)

C14—C15—C16—C12	−25.2 (3)	O312—C31—C32—C33	139.4 (2)
O12—C12—C16—C15	−77.4 (3)	O311—C31—C32—C33	−43.1 (3)
C11—C12—C16—C15	158.2 (2)	O32—C32—C33—C34	−96.4 (2)
C13—C12—C16—C15	37.1 (2)	C31—C32—C33—C34	141.41 (18)
O212—C21—C22—O22	−1.8 (3)	C36—C32—C33—C34	21.1 (2)
O211—C21—C22—O22	178.15 (17)	C32—C33—C34—C35	4.5 (2)
O212—C21—C22—C23	117.6 (2)	C33—C34—C35—C36	−28.5 (2)
O211—C21—C22—C23	−62.4 (2)	C34—C35—C36—C32	41.5 (2)
O212—C21—C22—C26	−125.9 (2)	O32—C32—C36—C35	76.1 (2)
O211—C21—C22—C26	54.0 (3)	C31—C32—C36—C35	−162.41 (17)
O22—C22—C23—C24	−79.8 (2)	C33—C32—C36—C35	−38.6 (2)
C21—C22—C23—C24	159.19 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O12—H12···O22^{i}	0.84	1.86	2.684 (2)	165
O111—H111···O112^{ii}	0.84	1.80	2.624 (2)	167
O22—H22···O32^{iii}	0.84	1.93	2.757 (2)	169
O211—H211···O212^{iv}	0.84	1.82	2.6559 (19)	177
O32—H32···O12^{v}	0.84	1.89	2.710 (2)	166
O311—H311···O312^{vi}	0.84	1.79	2.629 (2)	175

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

Fig. 1

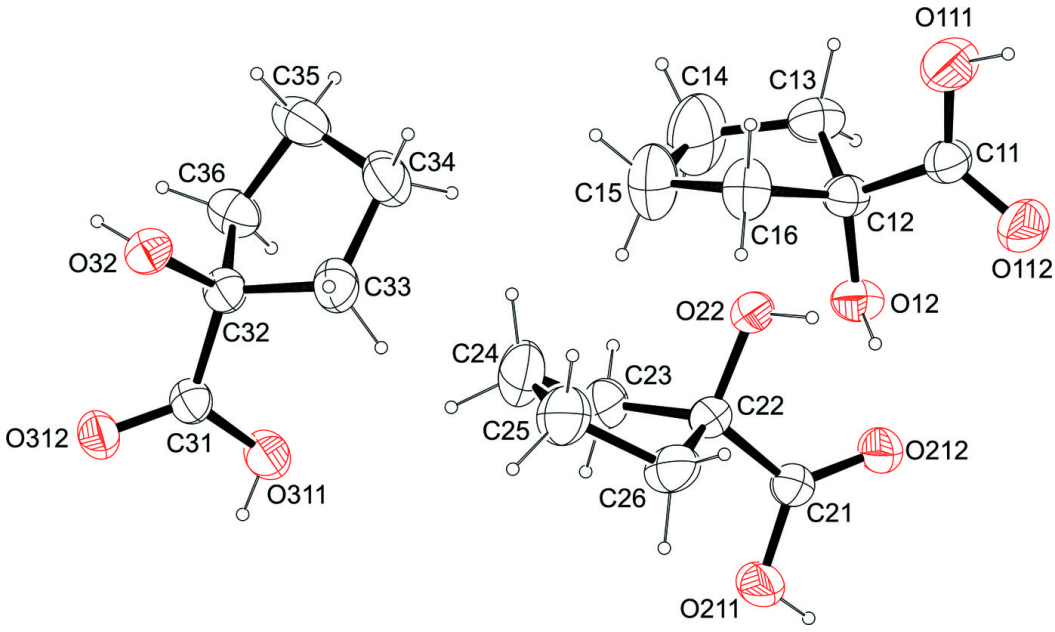
O111
C14
C13
C35
C11
C15
C34
C36
C16
C12
O112
O32
C33
O22
O12
C24
C32
C23
C22
O312
C31
C25
O212
O311
C26
C21
O211

Fig. 2