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The chalcone ethyl 2-[4-(2-[2,4-bis[(ethoxycarbonyl)methoxy]benzoyl]ethenyl)-phenoxy]acetate

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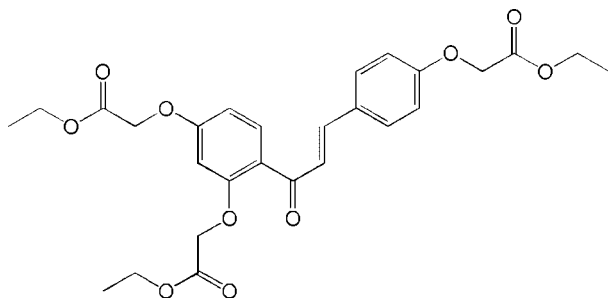
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.075; wR factor = 0.178; data-to-parameter ratio = 13.5.

In the title molecule, $\text{C}_{27}\text{H}_{30}\text{O}_{10}$, the benzene rings form a dihedral angle of $14.9(2)^\circ$. The $\text{C}=\text{C}$ bond is in an E conformation. In the crystal, weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds connect the molecules, forming a three-dimensional network.

Related literature

For a related structure, see: Wang *et al.* (2011).

Experimental

Crystal data

$\text{C}_{27}\text{H}_{30}\text{O}_{10}$
 $M_r = 514.51$
 Triclinic, $P\bar{1}$
 $a = 7.8225(16)$ Å
 $b = 13.579(3)$ Å

$c = 13.780(3)$ Å
 $\alpha = 63.004(3)^\circ$
 $\beta = 87.157(4)^\circ$
 $\gamma = 83.377(4)^\circ$
 $V = 1295.6(5)$ Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹

$T = 298$ K
 $0.12 \times 0.10 \times 0.10$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.988$, $T_{\max} = 0.990$

16520 measured reflections
 4538 independent reflections
 4137 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.075$
 $wR(F^2) = 0.178$
 $S = 1.20$
 4538 reflections

337 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.39$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3}\cdots\text{O1}^i$	0.93	2.52	3.276 (4)	138
$\text{C16}-\text{H16B}\cdots\text{O7}^{ii}$	0.97	2.58	3.337 (4)	135
$\text{C20}-\text{H20B}\cdots\text{O4}^{ii}$	0.97	2.60	3.360 (4)	136
$\text{C24}-\text{H24B}\cdots\text{O3}^{iii}$	0.97	2.53	3.339 (4)	141
$\text{C27}-\text{H27B}\cdots\text{O6}^{iv}$	0.96	2.56	3.426 (4)	150

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5675).

References

- Bruker (2004). APEX2 and SAINT. Bruker AXS Inc. Madison, Wisconsin, USA.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.
 Spek, A. L. (2009). Acta Cryst. D65, 148–155.
 Wang, J.-G., Wu, L., Zhong, C.-J., Ouyang, Z.-H. & Yi, D.-L. (2011). Acta Cryst. E67, o732.

supporting information

Acta Cryst. (2014). E70, o51 [https://doi.org/10.1107/S1600536813033114]

The chalcone ethyl 2-[4-(2-{2,4-bis[(ethoxycarbonyl)methoxy]benzoyl}-ethenyl)phenoxy]acetate

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S1. Comment

It has been determined in the authors lab that the title compound is a potential inhibitor of mushroom tyrosinase (results to be published soon) and the crystal structure determination of the title compound has been carried out to investigate its structure property relationships.

In the title molecule (I, Fig. 1) the two benzene rings (C10-C15/C1-C6) form a dihedral angle of 14.9 (2)°. The C=C bond is in an E conformation. In the crystal, weak C—H···O hydrogen bonds connect molecules forming a three-dimensional network (Fig. 2). The structure of a related compound, (E)-1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-prop-2-en-1-one monohydrate, has been published previously (Wang *et al.*, 2011).

S2. Experimental

Isoliquiritigenin (2.56 g, 0.01 mol) and potassium hydroxide (2.45 g, 0.0438 mol) were dissolved in dry acetone (100 ml) in a three-neck flask. Then ethyl bromoacetate (6.93 g, 0.0415 mol) was dropwise added at room temperature and vigorously stirred for 3 h. The progress of the reaction was monitored by TLC (Si gel, developing solvent *V* (ethyl acetate) / *V* (benzene) = 1:2). After suction filtration and distilled to remove the solvent, a light yellow solid was obtained, 4.39 g, yield 85.4%. Recrystallization from ethanol produced light yellow needles.

S3. Refinement

All hydrogen atoms were placed in ideal positions with the C—H = 0.93 Å, C—H = 0.96 Å and C—H = 0.97 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$.

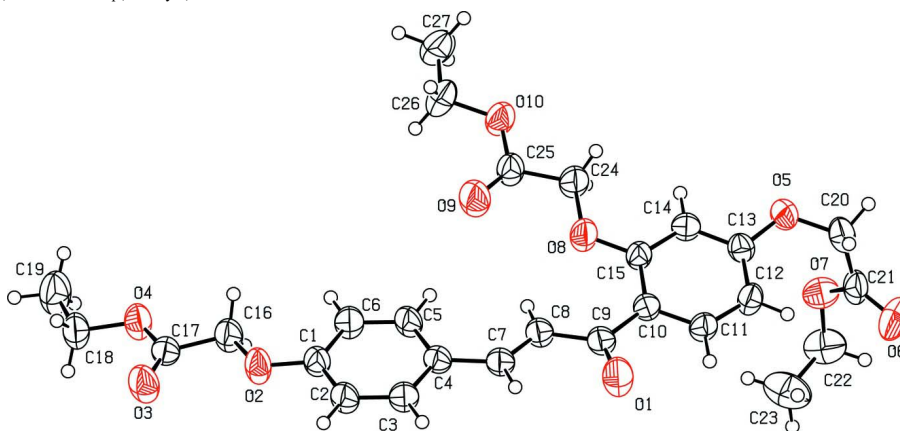


Figure 1

View of a molecule of (I) showing displacement ellipsoids drawn at the 50% probability level.

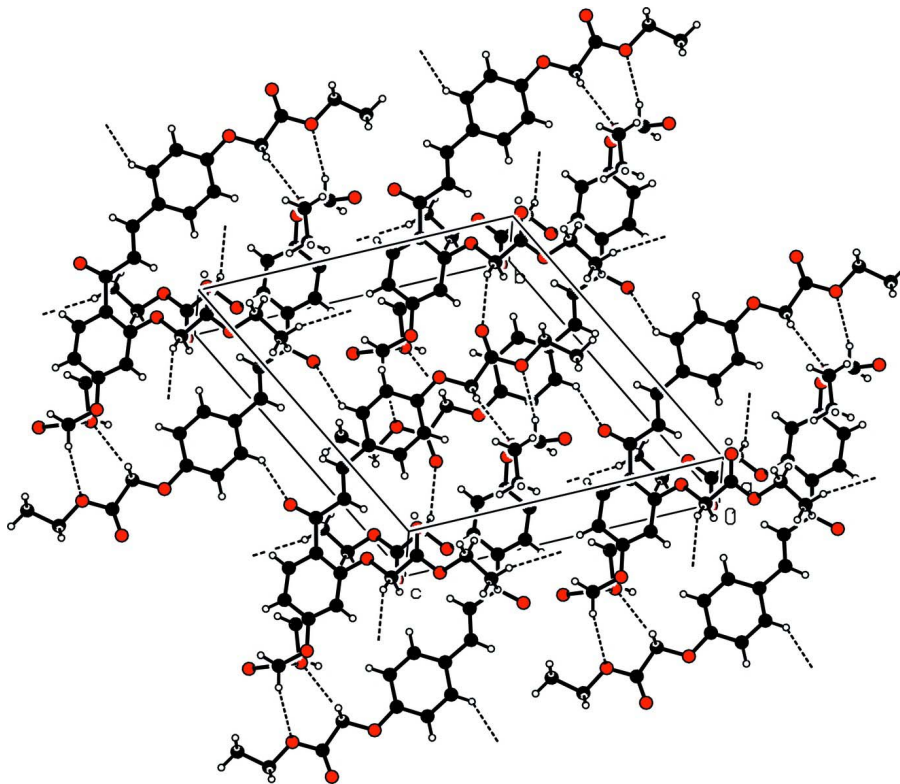


Figure 2

The crystal packing for (I), with weak C—H...O interactions shown as dashed lines.

Ethyl 2-[4-(2-{2,4-bis[(ethoxycarbonyl)methoxy]benzoyl}ethenyl)phenoxy]acetate

Crystal data

$C_{27}H_{30}O_{10}$

$M_r = 514.51$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 7.8225$ (16) Å

$b = 13.579$ (3) Å

$c = 13.780$ (3) Å

$\alpha = 63.004$ (3)°

$\beta = 87.157$ (4)°

$\gamma = 83.377$ (4)°

$V = 1295.6$ (5) Å³

$Z = 2$

$F(000) = 544$

$D_x = 1.319$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2402 reflections

$\theta = 0.0$ – 0.0 °

$\mu = 0.10$ mm⁻¹

$T = 298$ K

Block, light yellow

$0.12 \times 0.10 \times 0.10$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.988$, $T_{\max} = 0.990$

16520 measured reflections

4538 independent reflections

4137 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$
 $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 1.7^\circ$
 $h = -7 \rightarrow 9$

$k = -16 \rightarrow 16$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.075$
 $wR(F^2) = 0.178$
 $S = 1.20$
 4538 reflections
 337 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
 $w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 1.0739P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.39 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7304 (4)	0.4831 (2)	0.6468 (2)	0.0502 (7)
C2	0.7010 (4)	0.5453 (2)	0.7028 (2)	0.0549 (8)
H2	0.7100	0.6213	0.6670	0.066*
C3	0.6586 (4)	0.4962 (2)	0.8106 (2)	0.0532 (8)
H3	0.6387	0.5397	0.8471	0.064*
C4	0.6444 (4)	0.3821 (2)	0.8675 (2)	0.0456 (7)
C5	0.6802 (4)	0.3199 (2)	0.8103 (2)	0.0525 (7)
H5	0.6765	0.2434	0.8467	0.063*
C6	0.7211 (5)	0.3687 (2)	0.7015 (3)	0.0570 (8)
H6	0.7423	0.3258	0.6646	0.068*
C7	0.5925 (4)	0.3344 (2)	0.9813 (2)	0.0478 (7)
H7	0.5790	0.3829	1.0124	0.057*
C8	0.5619 (4)	0.2298 (2)	1.0465 (2)	0.0467 (7)
H8	0.5751	0.1776	1.0197	0.056*
C9	0.5081 (4)	0.1960 (2)	1.1589 (2)	0.0475 (7)
C10	0.4790 (4)	0.0787 (2)	1.2360 (2)	0.0415 (6)
C11	0.3962 (4)	0.0624 (2)	1.3330 (2)	0.0459 (7)
H11	0.3563	0.1246	1.3425	0.055*
C12	0.3700 (4)	-0.0400 (2)	1.4151 (2)	0.0485 (7)
H12	0.3136	-0.0470	1.4786	0.058*
C13	0.4293 (4)	-0.1333 (2)	1.4016 (2)	0.0435 (6)
C14	0.5085 (4)	-0.1219 (2)	1.3063 (2)	0.0463 (7)

H14	0.5449	-0.1848	1.2970	0.056*
C15	0.5343 (4)	-0.0178 (2)	1.2239 (2)	0.0432 (6)
C16	0.7769 (5)	0.4821 (2)	0.4757 (2)	0.0587 (8)
H16A	0.6704	0.4490	0.4833	0.070*
H16B	0.8709	0.4230	0.5006	0.070*
C17	0.8034 (4)	0.5619 (2)	0.3588 (2)	0.0517 (7)
C18	0.8388 (5)	0.5709 (3)	0.1834 (2)	0.0623 (9)
H18A	0.9452	0.6053	0.1695	0.075*
H18B	0.7445	0.6287	0.1514	0.075*
C19	0.8467 (6)	0.4911 (3)	0.1360 (3)	0.0855 (12)
H19A	0.9402	0.4342	0.1687	0.128*
H19B	0.8644	0.5300	0.0589	0.128*
H19C	0.7405	0.4579	0.1501	0.128*
C20	0.3347 (4)	-0.2565 (3)	1.5781 (2)	0.0563 (8)
H20A	0.3860	-0.2134	1.6068	0.068*
H20B	0.3559	-0.3343	1.6303	0.068*
C21	0.1446 (5)	-0.2243 (2)	1.5680 (2)	0.0547 (8)
C22	-0.0998 (5)	-0.1807 (3)	1.4570 (4)	0.0775 (11)
H22A	-0.1640	-0.1962	1.5235	0.093*
H22B	-0.1500	-0.2159	1.4194	0.093*
C23	-0.1101 (6)	-0.0602 (3)	1.3875 (4)	0.0955 (14)
H23A	-0.0536	-0.0262	1.4231	0.143*
H23B	-0.2287	-0.0300	1.3748	0.143*
H23C	-0.0548	-0.0455	1.3192	0.143*
C24	0.6858 (5)	-0.0966 (2)	1.1165 (3)	0.0592 (8)
H24A	0.5934	-0.1392	1.1180	0.071*
H24B	0.7663	-0.1441	1.1747	0.071*
C25	0.7749 (4)	-0.0555 (3)	1.0089 (2)	0.0522 (7)
C26	0.9388 (5)	-0.1206 (3)	0.8969 (3)	0.0672 (9)
H26A	1.0458	-0.0924	0.8998	0.081*
H26B	0.8735	-0.0652	0.8340	0.081*
C27	0.9746 (5)	-0.2257 (3)	0.8881 (3)	0.0744 (10)
H27A	1.0383	-0.2802	0.9509	0.112*
H27B	1.0409	-0.2128	0.8236	0.112*
H27C	0.8680	-0.2523	0.8839	0.112*
O1	0.4841 (4)	0.26559 (18)	1.19312 (19)	0.0826 (9)
O2	0.7698 (3)	0.54015 (16)	0.53900 (17)	0.0655 (7)
O3	0.8152 (4)	0.65850 (18)	0.32433 (19)	0.0776 (8)
O4	0.8129 (3)	0.50759 (17)	0.29960 (16)	0.0608 (6)
O5	0.4174 (3)	-0.24062 (16)	1.47859 (16)	0.0541 (5)
O6	0.0654 (4)	-0.2021 (3)	1.6330 (2)	0.0971 (10)
O7	0.0789 (3)	-0.22501 (18)	1.48300 (19)	0.0618 (6)
O8	0.6192 (3)	-0.00224 (16)	1.13008 (17)	0.0653 (7)
O9	0.7865 (4)	0.03736 (19)	0.9457 (2)	0.0800 (8)
O10	0.8417 (3)	-0.14310 (17)	0.99470 (18)	0.0649 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0668 (19)	0.0382 (15)	0.0429 (15)	-0.0079 (13)	0.0095 (13)	-0.0164 (13)
C2	0.084 (2)	0.0296 (14)	0.0496 (17)	-0.0093 (14)	0.0116 (15)	-0.0164 (13)
C3	0.077 (2)	0.0357 (15)	0.0514 (17)	-0.0058 (14)	0.0095 (15)	-0.0243 (14)
C4	0.0550 (17)	0.0351 (14)	0.0448 (15)	-0.0043 (12)	0.0028 (13)	-0.0167 (12)
C5	0.077 (2)	0.0294 (14)	0.0467 (16)	-0.0097 (13)	0.0093 (14)	-0.0137 (12)
C6	0.087 (2)	0.0378 (15)	0.0510 (17)	-0.0099 (15)	0.0129 (16)	-0.0245 (14)
C7	0.0630 (18)	0.0347 (14)	0.0464 (16)	-0.0035 (13)	0.0047 (13)	-0.0198 (13)
C8	0.0611 (18)	0.0381 (15)	0.0424 (15)	-0.0054 (13)	0.0022 (13)	-0.0195 (12)
C9	0.0638 (19)	0.0367 (14)	0.0436 (15)	-0.0035 (13)	0.0021 (13)	-0.0202 (13)
C10	0.0482 (16)	0.0381 (14)	0.0398 (14)	-0.0039 (11)	0.0011 (12)	-0.0191 (12)
C11	0.0592 (18)	0.0397 (15)	0.0457 (15)	-0.0066 (13)	0.0067 (13)	-0.0257 (13)
C12	0.0607 (18)	0.0477 (16)	0.0422 (15)	-0.0140 (13)	0.0145 (13)	-0.0242 (13)
C13	0.0474 (16)	0.0383 (14)	0.0421 (15)	-0.0092 (12)	0.0025 (12)	-0.0150 (12)
C14	0.0580 (18)	0.0355 (14)	0.0486 (16)	-0.0049 (12)	0.0045 (13)	-0.0222 (13)
C15	0.0545 (17)	0.0392 (14)	0.0379 (14)	-0.0053 (12)	0.0060 (12)	-0.0196 (12)
C16	0.088 (2)	0.0410 (16)	0.0473 (17)	-0.0109 (15)	0.0127 (16)	-0.0206 (14)
C17	0.067 (2)	0.0381 (16)	0.0475 (16)	-0.0028 (13)	0.0083 (14)	-0.0183 (13)
C18	0.085 (2)	0.0570 (19)	0.0402 (16)	-0.0134 (17)	0.0100 (15)	-0.0179 (15)
C19	0.126 (4)	0.080 (3)	0.057 (2)	-0.022 (2)	0.017 (2)	-0.037 (2)
C20	0.077 (2)	0.0471 (17)	0.0390 (15)	-0.0150 (15)	0.0043 (15)	-0.0130 (13)
C21	0.079 (2)	0.0411 (16)	0.0405 (16)	-0.0178 (15)	0.0179 (15)	-0.0143 (13)
C22	0.066 (2)	0.069 (2)	0.105 (3)	-0.0102 (18)	-0.001 (2)	-0.045 (2)
C23	0.076 (3)	0.072 (3)	0.122 (4)	-0.001 (2)	-0.025 (3)	-0.028 (3)
C24	0.086 (2)	0.0410 (16)	0.0536 (18)	-0.0068 (15)	0.0161 (16)	-0.0254 (14)
C25	0.070 (2)	0.0463 (17)	0.0440 (16)	-0.0119 (14)	0.0091 (14)	-0.0231 (14)
C26	0.071 (2)	0.081 (2)	0.063 (2)	-0.0145 (18)	0.0210 (17)	-0.0441 (19)
C27	0.080 (3)	0.085 (3)	0.071 (2)	0.000 (2)	0.0112 (19)	-0.049 (2)
O1	0.149 (3)	0.0424 (12)	0.0593 (14)	-0.0150 (14)	0.0280 (15)	-0.0274 (11)
O2	0.1146 (19)	0.0361 (11)	0.0445 (12)	-0.0161 (11)	0.0222 (12)	-0.0174 (9)
O3	0.133 (2)	0.0401 (13)	0.0555 (14)	-0.0114 (13)	0.0162 (14)	-0.0190 (11)
O4	0.0943 (17)	0.0451 (12)	0.0437 (11)	-0.0165 (11)	0.0133 (11)	-0.0197 (10)
O5	0.0667 (14)	0.0383 (11)	0.0483 (12)	-0.0082 (9)	0.0106 (10)	-0.0121 (9)
O6	0.114 (2)	0.114 (2)	0.0670 (17)	-0.0088 (18)	0.0327 (16)	-0.0479 (17)
O7	0.0630 (14)	0.0582 (13)	0.0735 (15)	-0.0026 (11)	-0.0009 (11)	-0.0387 (12)
O8	0.1049 (18)	0.0377 (11)	0.0509 (12)	-0.0062 (11)	0.0263 (12)	-0.0208 (10)
O9	0.124 (2)	0.0459 (14)	0.0626 (15)	-0.0082 (13)	0.0233 (15)	-0.0203 (12)
O10	0.0907 (17)	0.0486 (12)	0.0585 (13)	-0.0094 (11)	0.0247 (12)	-0.0288 (11)

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

C1—O2	1.366 (3)	C17—O4	1.319 (4)
C1—C2	1.375 (4)	C18—O4	1.450 (4)
C1—C6	1.394 (4)	C18—C19	1.492 (5)
C2—C3	1.365 (4)	C18—H18A	0.9700
C2—H2	0.9300	C18—H18B	0.9700

C3—C4	1.399 (4)	C19—H19A	0.9600
C3—H3	0.9300	C19—H19B	0.9600
C4—C5	1.393 (4)	C19—H19C	0.9600
C4—C7	1.455 (4)	C20—O5	1.422 (4)
C5—C6	1.375 (4)	C20—C21	1.496 (5)
C5—H5	0.9300	C20—H20A	0.9700
C6—H6	0.9300	C20—H20B	0.9700
C7—C8	1.335 (4)	C21—O6	1.193 (4)
C7—H7	0.9300	C21—O7	1.307 (4)
C8—C9	1.457 (4)	C22—O7	1.451 (4)
C8—H8	0.9300	C22—C23	1.468 (5)
C9—O1	1.227 (3)	C22—H22A	0.9700
C9—C10	1.497 (4)	C22—H22B	0.9700
C10—C11	1.389 (4)	C23—H23A	0.9600
C10—C15	1.412 (4)	C23—H23B	0.9600
C11—C12	1.368 (4)	C23—H23C	0.9600
C11—H11	0.9300	C24—O8	1.415 (3)
C12—C13	1.387 (4)	C24—C25	1.494 (4)
C12—H12	0.9300	C24—H24A	0.9700
C13—O5	1.370 (3)	C24—H24B	0.9700
C13—C14	1.375 (4)	C25—O9	1.174 (4)
C14—C15	1.384 (4)	C25—O10	1.335 (4)
C14—H14	0.9300	C26—O10	1.437 (4)
C15—O8	1.363 (3)	C26—C27	1.481 (5)
C16—O2	1.412 (3)	C26—H26A	0.9700
C16—C17	1.499 (4)	C26—H26B	0.9700
C16—H16A	0.9700	C27—H27A	0.9600
C16—H16B	0.9700	C27—H27B	0.9600
C17—O3	1.189 (3)	C27—H27C	0.9600
O2—C1—C2	116.0 (2)	O4—C18—H18B	110.3
O2—C1—C6	124.5 (3)	C19—C18—H18B	110.3
C2—C1—C6	119.5 (3)	H18A—C18—H18B	108.6
C3—C2—C1	120.5 (3)	C18—C19—H19A	109.5
C3—C2—H2	119.8	C18—C19—H19B	109.5
C1—C2—H2	119.8	H19A—C19—H19B	109.5
C2—C3—C4	121.5 (3)	C18—C19—H19C	109.5
C2—C3—H3	119.2	H19A—C19—H19C	109.5
C4—C3—H3	119.2	H19B—C19—H19C	109.5
C5—C4—C3	117.1 (3)	O5—C20—C21	114.2 (3)
C5—C4—C7	123.4 (2)	O5—C20—H20A	108.7
C3—C4—C7	119.5 (2)	C21—C20—H20A	108.7
C6—C5—C4	121.7 (3)	O5—C20—H20B	108.7
C6—C5—H5	119.1	C21—C20—H20B	108.7
C4—C5—H5	119.1	H20A—C20—H20B	107.6
C5—C6—C1	119.6 (3)	O6—C21—O7	125.4 (4)
C5—C6—H6	120.2	O6—C21—C20	121.9 (3)
C1—C6—H6	120.2	O7—C21—C20	112.7 (3)

C8—C7—C4	128.1 (3)	O7—C22—C23	109.5 (3)
C8—C7—H7	116.0	O7—C22—H22A	109.8
C4—C7—H7	116.0	C23—C22—H22A	109.8
C7—C8—C9	121.0 (3)	O7—C22—H22B	109.8
C7—C8—H8	119.5	C23—C22—H22B	109.8
C9—C8—H8	119.5	H22A—C22—H22B	108.2
O1—C9—C8	119.6 (3)	C22—C23—H23A	109.5
O1—C9—C10	117.6 (3)	C22—C23—H23B	109.5
C8—C9—C10	122.8 (2)	H23A—C23—H23B	109.5
C11—C10—C15	116.3 (2)	C22—C23—H23C	109.5
C11—C10—C9	116.4 (2)	H23A—C23—H23C	109.5
C15—C10—C9	127.2 (2)	H23B—C23—H23C	109.5
C12—C11—C10	123.8 (3)	O8—C24—C25	107.2 (2)
C12—C11—H11	118.1	O8—C24—H24A	110.3
C10—C11—H11	118.1	C25—C24—H24A	110.3
C11—C12—C13	118.5 (3)	O8—C24—H24B	110.3
C11—C12—H12	120.7	C25—C24—H24B	110.3
C13—C12—H12	120.7	H24A—C24—H24B	108.5
O5—C13—C14	115.1 (2)	O9—C25—O10	124.3 (3)
O5—C13—C12	124.6 (2)	O9—C25—C24	127.2 (3)
C14—C13—C12	120.2 (2)	O10—C25—C24	108.5 (2)
C13—C14—C15	120.6 (2)	O10—C26—C27	108.1 (3)
C13—C14—H14	119.7	O10—C26—H26A	110.1
C15—C14—H14	119.7	C27—C26—H26A	110.1
O8—C15—C14	122.9 (2)	O10—C26—H26B	110.1
O8—C15—C10	116.4 (2)	C27—C26—H26B	110.1
C14—C15—C10	120.6 (2)	H26A—C26—H26B	108.4
O2—C16—C17	108.9 (2)	C26—C27—H27A	109.5
O2—C16—H16A	109.9	C26—C27—H27B	109.5
C17—C16—H16A	109.9	H27A—C27—H27B	109.5
O2—C16—H16B	109.9	C26—C27—H27C	109.5
C17—C16—H16B	109.9	H27A—C27—H27C	109.5
H16A—C16—H16B	108.3	H27B—C27—H27C	109.5
O3—C17—O4	125.1 (3)	C1—O2—C16	117.3 (2)
O3—C17—C16	125.8 (3)	C17—O4—C18	117.4 (2)
O4—C17—C16	109.1 (2)	C13—O5—C20	117.2 (2)
O4—C18—C19	106.9 (3)	C21—O7—C22	117.3 (3)
O4—C18—H18A	110.3	C15—O8—C24	118.7 (2)
C19—C18—H18A	110.3	C25—O10—C26	116.9 (3)
O2—C1—C2—C3	179.2 (3)	C11—C10—C15—O8	-178.5 (3)
C6—C1—C2—C3	-1.7 (5)	C9—C10—C15—O8	-2.1 (4)
C1—C2—C3—C4	0.3 (5)	C11—C10—C15—C14	-1.1 (4)
C2—C3—C4—C5	1.8 (5)	C9—C10—C15—C14	175.2 (3)
C2—C3—C4—C7	-177.7 (3)	O2—C16—C17—O3	-0.6 (5)
C3—C4—C5—C6	-2.6 (5)	O2—C16—C17—O4	179.0 (3)
C7—C4—C5—C6	176.9 (3)	O5—C20—C21—O6	-158.1 (3)
C4—C5—C6—C1	1.3 (5)	O5—C20—C21—O7	22.8 (4)

O2—C1—C6—C5	180.0 (3)	O8—C24—C25—O9	-1.1 (5)
C2—C1—C6—C5	0.9 (5)	O8—C24—C25—O10	179.0 (3)
C5—C4—C7—C8	-3.9 (5)	C2—C1—O2—C16	-171.3 (3)
C3—C4—C7—C8	175.5 (3)	C6—C1—O2—C16	9.6 (5)
C4—C7—C8—C9	-179.1 (3)	C17—C16—O2—C1	174.2 (3)
C7—C8—C9—O1	2.8 (5)	O3—C17—O4—C18	-0.3 (5)
C7—C8—C9—C10	-177.6 (3)	C16—C17—O4—C18	-179.9 (3)
O1—C9—C10—C11	11.9 (4)	C19—C18—O4—C17	179.4 (3)
C8—C9—C10—C11	-167.7 (3)	C14—C13—O5—C20	-179.2 (3)
O1—C9—C10—C15	-164.5 (3)	C12—C13—O5—C20	1.5 (4)
C8—C9—C10—C15	15.9 (5)	C21—C20—O5—C13	70.3 (3)
C15—C10—C11—C12	1.3 (4)	O6—C21—O7—C22	9.1 (5)
C9—C10—C11—C12	-175.5 (3)	C20—C21—O7—C22	-171.9 (3)
C10—C11—C12—C13	0.1 (5)	C23—C22—O7—C21	87.1 (4)
C11—C12—C13—O5	177.5 (3)	C14—C15—O8—C24	-0.8 (5)
C11—C12—C13—C14	-1.7 (4)	C10—C15—O8—C24	176.5 (3)
O5—C13—C14—C15	-177.4 (3)	C25—C24—O8—C15	-178.7 (3)
C12—C13—C14—C15	1.9 (4)	O9—C25—O10—C26	2.3 (5)
C13—C14—C15—O8	176.8 (3)	C24—C25—O10—C26	-177.7 (3)
C13—C14—C15—C10	-0.4 (4)	C27—C26—O10—C25	-170.4 (3)

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>
C3—H3...O1 ⁱ	0.93	2.52	3.276 (4)	138
C16—H16 <i>B</i> ...O7 ⁱⁱ	0.97	2.58	3.337 (4)	135
C20—H20 <i>B</i> ...O4 ⁱⁱ	0.97	2.60	3.360 (4)	136
C24—H24 <i>B</i> ...O3 ⁱⁱⁱ	0.97	2.53	3.339 (4)	141
C27—H27 <i>B</i> ...O6 ^{iv}	0.96	2.56	3.426 (4)	150

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