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Crystal structures and Hirshfeld surface analyses of diphenylmethyl 2-(3,5-dimethoxyphenyl)acetate and diphenylmethyl 2-(3,4,5-trimethoxyphenyl)-acetate

Manivel Kavitha,[a] Chandiran Jayakodi,[a] Ganesan Meenambigai,[a] Sekar Janarthanan,[a] Srinivasan Pazhamalai[a]* and Sivashanmugam Selvanayagam[b]‡

[a]Department of Chemistry, Annamalai University, Annamalainagar, Chidambaram 608 002, India, and [b]PG & Research Department of Physics, Government Arts College, Melur 625 106, India. *Correspondence e-mail: sripazhamalai@gmail.com

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‡ Additional correspondence author, e-mail: sselvanayagam@gmail.com.

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CCDC references: 2400579; 2400580

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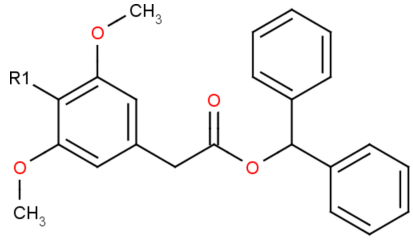
The title compounds, $C_{23}H_{22}O_4$, (I), and $C_{24}H_{24}O_5$, (II), differ in the presence of a methoxy group instead of a hydrogen atom between two methoxy groups attached to the phenyl ring of the phenyl acetate moiety, which affects not only the symmetry and number of formula units [triclinic, $P\overline{1}$, $Z = 2$ for (I); monoclinic, $P2_1/n$, $Z = 4$ for (II)], but also the molecular conformations. An overlay of the two molecular structures reveals a large root-mean-square-deviation of 2.4 Å. Intra and intermolecular C—H···O hydrogen bonds are responsible for the consolidation of the molecular conformations and the crystal packing of both structures. Their intermolecular interactions were quantified and analysed using Hirshfeld surface analysis, revealing that H···H interactions contribute most to the crystal packing.

1. Chemical context

Esters are fundamental synthons or synthetic targets, as they are widely found in bioactive natural compounds and thus are important in both pharmaceutical and industrial applications. Esterifications are typically carried out under mild conditions, making them suitable for the synthesis of sensitive and labile compounds (Chiodi & Ishihara, 2024).

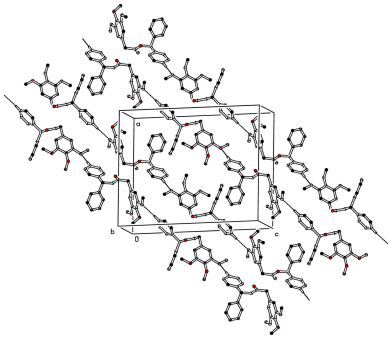


R1 - H in (I) and OCH_3 in (II)

In the present work, the synthesis, structural and Hirshfeld surface analysis of the esters diphenylmethyl 2-(3,5-dimethoxyphenyl)acetate, (I), and diphenylmethyl-2-(3,4,5-trimethoxyphenyl)acetate, (II), are reported.

2. Structural commentary

The molecular structures of (I) and (II) are illustrated in Figs. 1 and 2. Although the two molecules differ only in the presence of a methoxy group instead of a hydrogen atom in between two methoxy groups, they adopt different conformations, as an overlay plot of the two molecules shows (Fig. 3);



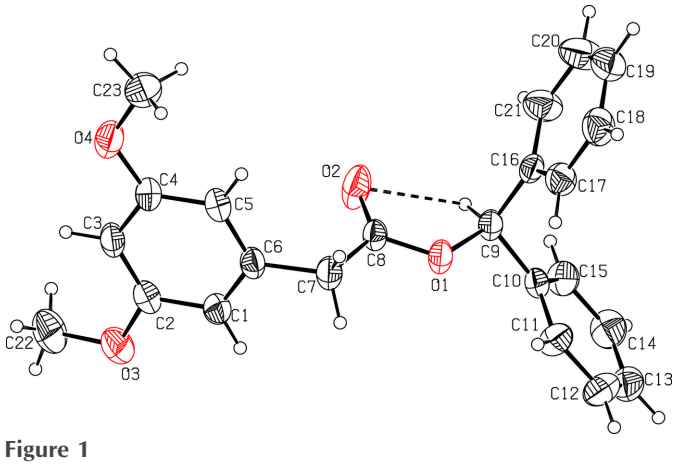


Figure 1
The molecular structure of compound (I) with displacement ellipsoids drawn at the 30% probability level. The intramolecular C—H···O interaction is shown as a dashed line.

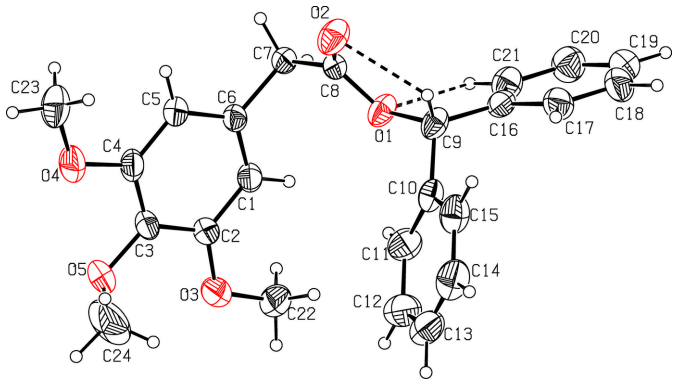


Figure 2
The molecular structure of compound (II) with displacement ellipsoids drawn at the 30% probability level. Intramolecular C—H···O interactions are shown as dashed lines.

the root-mean-square-deviation is 2.4 Å. The dimethoxy phenyl ring in (I) is planar with a maximum deviation of −0.005 (3) Å for atom C1 and its attached atoms of the methoxy groups (O3, C22; O4, C23) deviate by 0.015 (2), 0.228 (4), −0.020 (2) and 0.005 (4) Å, respectively, from this plane. The acetate moiety (C7/C8/O1/C9/O2) in (I) is nearly planar with a maximum deviation of −0.110 (2) Å for atom O2 from the best plane. This moiety forms a dihedral angle of 83.7 (1)° with respect to the dimethoxy phenyl ring. The two phenyl rings (C10–C15; C16–C21) of the diphenylmethyl moiety in (I) are oriented at a dihedral angle of 71.1 (2)°.

The trimethoxy phenyl ring in (II) is planar with a maximum deviation of 0.007 (2) Å for atom C1 and its attached methoxy atoms (O3, C22; O4, C23; O5 C24) deviate by 0.015 (2), 0.038 (3), 0.031 (2), −0.067 (3), 0.076 (2) and −1.165 (5) Å, respectively, from this plane. The acetate moiety (C7/C8/O1/C9/O2) in (II) is planar with a maximum deviation of 0.005 (2) Å for atom C9. This moiety forms a dihedral angle of 71.4 (1)° with respect to the trimethoxy phenyl ring. The two phenyl rings (C10–C15; C16–C21) in (II) are oriented at a dihedral angle of 65.6 (2)°.

Weak intramolecular C—H···O hydrogen bonds between the methine H atom of the diphenylmethyl entity consolidate the molecular conformation in both cases (Figs. 1, 2; Tables 1, 2).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2	0.98	2.30	2.667 (3)	101
C9—H9···O2^{i}	0.98	2.50	3.444 (3)	162

Symmetry code: (i) $-x, -y+2, -z+1$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2	0.98	2.24	2.691 (3)	107
C21—H21···O1	0.93	2.39	2.740 (3)	102
C19—H19···O4^{i}	0.93	2.50	3.427 (3)	175

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

3. Supramolecular features

In the crystal of (I), molecules associate pairwise *via* C9—H9···O2^{i} hydrogen bonds (Table 1) into inversion dimers with an $R_2^2(10)$ graph-set motif (Etter *et al.*, 1990), as shown in

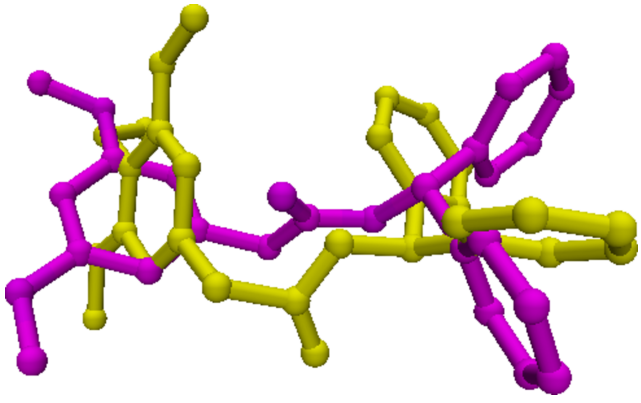


Figure 3
Superposition of molecules (I) (violet) and (II) (yellow), except for the methoxy group [O5–C24 in (II)]. The overlay plot was produced with *Qmol* (Gans & Shalloway, 2001).

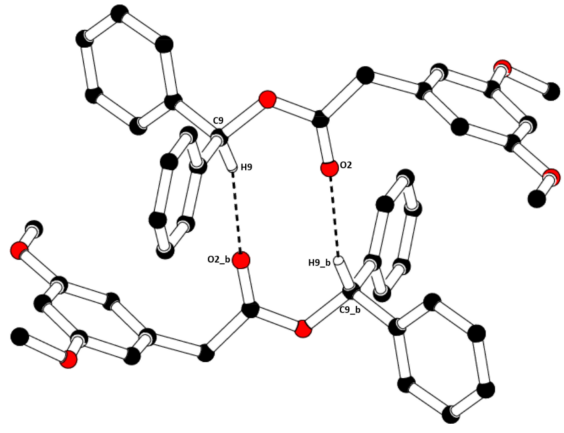


Figure 4
The formation of a centrosymmetric dimer in the crystal structure of (I) through C—H···O hydrogen bonds (dashed lines). [Symmetry code: (*b*) $-x, -y+2, -z+1$]

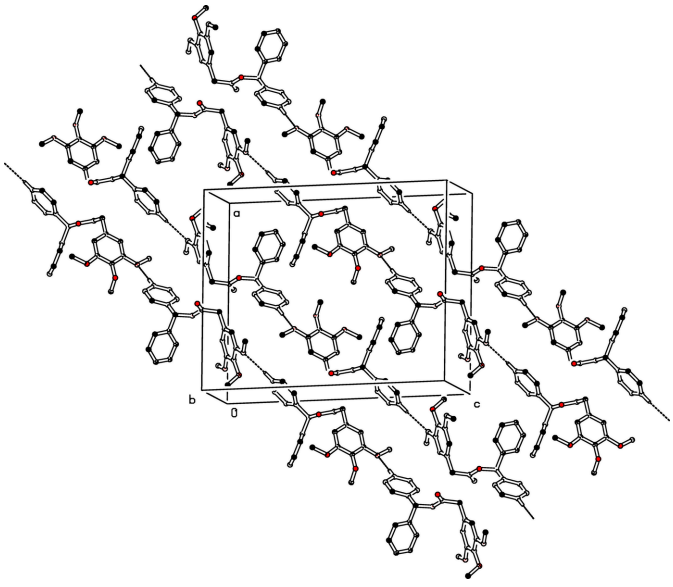


Figure 5
The crystal packing of (II) viewed approximately down the *b* axis. C—H···O intermolecular hydrogen bonds are shown as dashed lines; for clarity H atoms not involved in these hydrogen bonds have been omitted.

Fig. 4. In the crystal of (II), molecules associate into a *C*(13) chain by C19—H19···O4^{i} hydrogen bonds running in anti-parallel manner along [101] (Table 2; Fig. 5).

4. Hirshfeld surface analysis

To further characterize the intermolecular interactions in the title compound, a Hirshfeld surface (HS) analysis (Spackman & Jayatilaka, 2009) was carried out with *CrystalExplorer* (Spackman *et al.*, 2021). The HS mapped over d_{norm} for (I) and (II) are illustrated in Figs. 6 and 7, respectively, with a colour scheme to indicate contacts shorter (red areas), equal to (white areas), or longer than (blue areas) the sum of the van der Waals radii (Ashfaq *et al.*, 2021).

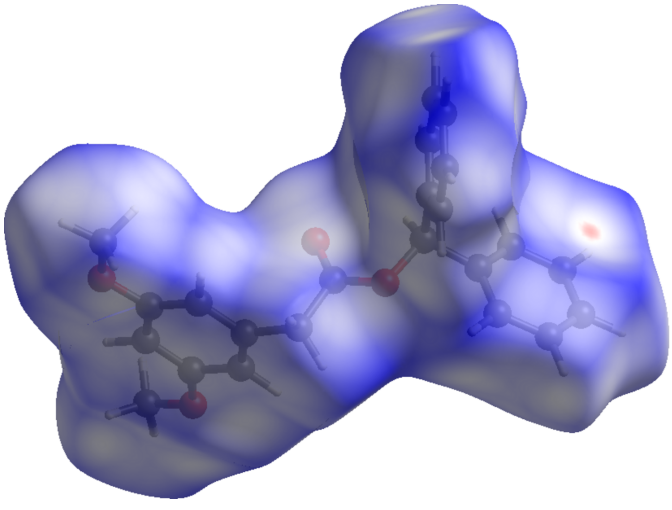


Figure 6
A view of the Hirshfeld surface mapped over d_{norm} for (I).

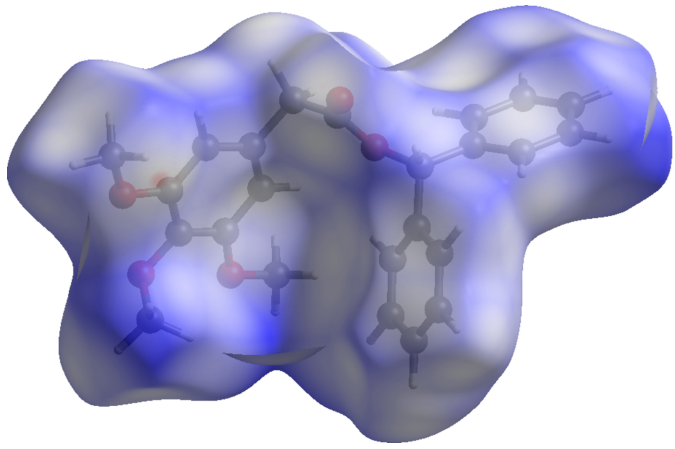


Figure 7
A view of the Hirshfeld surface mapped over d_{norm} for (II).

The associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) provide quantitative information about the non-covalent interactions in the crystal packing in terms of the percentage contribution of the interatomic contacts (Spackman & McKinnon, 2002). The overall two-dimensional fingerprint plot for compound (I) is shown in Fig. 8*a*. H···H and H···C/C···H contacts are the main contributors to the crystal packing, followed by H···O/O···H,

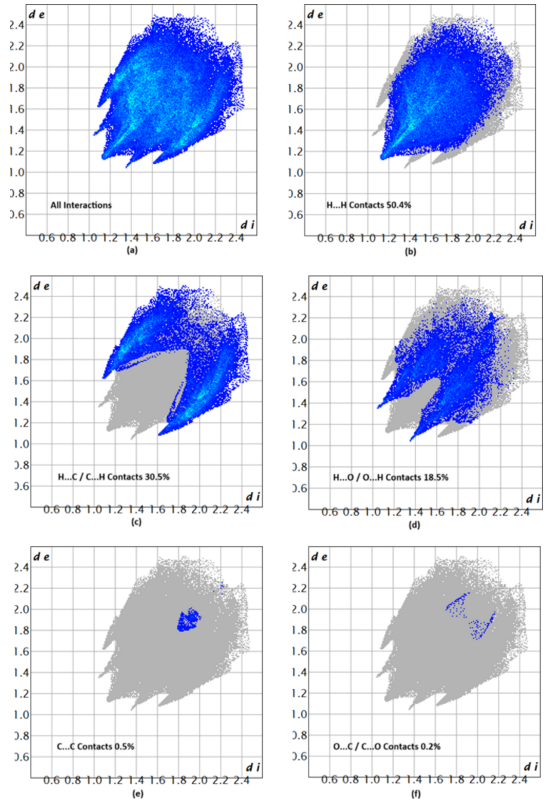


Figure 8
Two-dimensional fingerprint plots for (I), showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···C/C···H, (*d*) H···O/O···H, (*e*) C···C and (*f*) O···C/C···O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{23}H_{22}O_4$	$C_{24}H_{24}O_5$
M_r	362.40	392.43
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$
Temperature (K)	300	300
a, b, c (Å)	8.5327 (12), 11.0216 (15), 11.4369 (16)	17.2290 (14), 5.5037 (5), 22.1140 (18)
α, β, γ (°)	111.817 (4), 96.977 (4), 99.925 (4)	90, 92.256 (2), 90
V (Å^3)	963.1 (2)	2095.3 (3)
Z	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.09	0.09
Crystal size (mm)	0.19 × 0.18 × 0.17	0.28 × 0.09 × 0.07
Data collection		
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.674, 0.746	0.694, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24070, 4782, 2717	39211, 5016, 2516
R_{int}	0.047	0.074
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668	0.660
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.202, 1.04	0.057, 0.176, 1.00
No. of reflections	4782	5016
No. of parameters	245	263
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.68, −0.45	0.25, −0.18

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT* (Sheldrick, 2015*a*), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2020) and *SHELXL* (Sheldrick, 2015*b*).

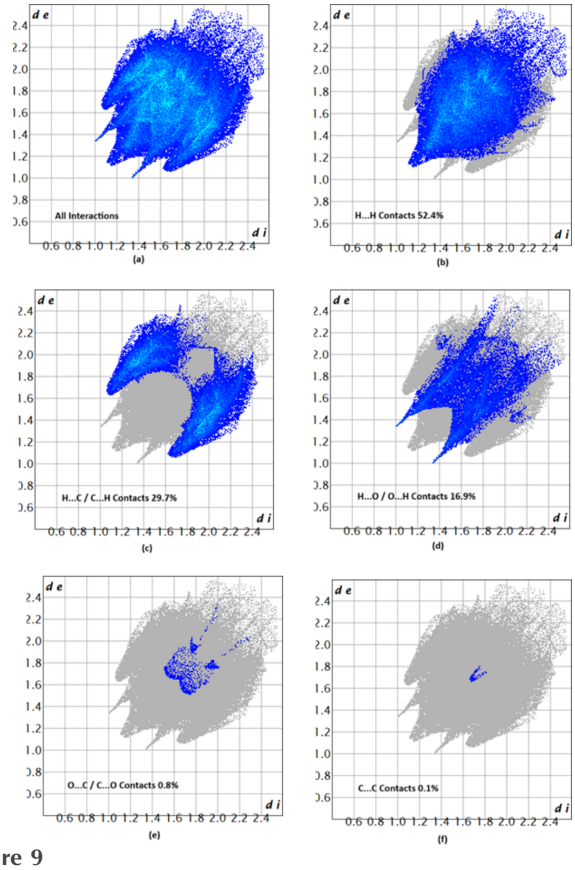


Figure 9
Two-dimensional fingerprint plots for compound (II), showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···C/C···H, (*d*) H···O/O···H, (*e*) O···C/C···O and (*f*) C···C interactions.

C···C and O···C/C···O contacts for compound (I), as shown in Fig. 8*b–f*. In compound (II), the overall two-dimensional fingerprint is shown in Fig. 9*a*. Again, H···H and H···C/C···H contacts are the main contributors to the crystal packing, followed by H···O/O···H, O···C/C···O and C···C contacts (Fig. 9*b–f*). The HS analysis confirms the importance of H-atom contacts in establishing the packing (Hathwar *et al.*, 2015).

5. Synthesis and crystallization

For the synthesis of (I), a mixture containing 3,5-dimethoxyphenylacetic acid (0.1 mmol), benzhydrol (0.1 mmol), *N*,*N*′-dicyclohexylcarbodiimide (0.4 g), and 4-dimethylaminopyridine (0.8 g) was placed into a 250 ml round-bottom flask. To this, 100 ml of dichloromethane were added, and the reaction mixture was refluxed on a water bath at 321 K for 9–11 h. After completion of the reaction, as monitored by thin-layer chromatography (TLC), the precipitate formed was filtered off, and the solvent was evaporated to dryness. The crude product was then purified by column chromatography using a solvent system of ethyl acetate and petroleum ether in a 1:4 (*v*:*v*) ratio. The separated product was dried *in vacuo*, giving colourless crystals with 85% yield.

For the synthesis of (II), a mixture containing 3,4,5-dimethoxyphenylacetic acid (0.1 mmol), benzhydrol (0.1 mmol), *N*,*N*′-dicyclohexylcarbodiimide (0.4 g), and 4-dimethylaminopyridine (0.8 g) was placed into a 250 ml round-bottom flask. To this, 100 ml of dichloromethane was added, and the reac-

tion mixture was refluxed on a water bath at 321 K for 9–11 h. Upon completion of the reaction, as monitored by thin-layer chromatography (TLC), the precipitate formed was filtered off, and the solvent was evaporated to dryness. The crude product was then purified by column chromatography using a solvent system of ethyl acetate and petroleum ether in a 1:4 (*v*:*v*) ratio. The resulting compound was obtained as colourless crystals with a 90% yield.

For (I) and (II), the solid products were recrystallized from methanol to obtain crystals suitable for X-ray analysis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. In both (I) and (II), H atoms were placed in idealized positions and allowed to ride on their parent atoms: C—H = 0.93–0.98 Å, with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C) for other H atoms.

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Crystal structures and Hirshfeld surface analyses of diphenylmethyl 2-(3,5-dimethoxyphenyl)acetate and diphenylmethyl 2-(3,4,5-trimethoxyphenyl)acetate

Manivel Kavitha, Chandiran Jayakodi, Ganesan Meenambigai, Sekar Janarthanan, Srinivasan Pazhamalai and Sivashanmugam Selvanayagam

Computing details

Diphenylmethyl 2-(3,5-dimethoxyphenyl)acetate (I)

Crystal data

$C_{23}H_{22}O_4$
M_r = 362.40
Triclinic, $P\overline{1}$
a = 8.5327 (12) Å
b = 11.0216 (15) Å
c = 11.4369 (16) Å
α = 111.817 (4)°
β = 96.977 (4)°
γ = 99.925 (4)°
V = 963.1 (2) Å^3
Z = 2
$F(000)$ = 384
D_x = 1.250 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6939 reflections
θ = 2.5–24.7°
μ = 0.09 mm^{-1}
T = 300 K
Block, colourless
0.19 × 0.18 × 0.17 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: i-mu-s microfocus source
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.674, T_{max} = 0.746
24070 measured reflections
4782 independent reflections
2717 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 28.3°, θ_{min} = 2.0°
h = −11→11
k = −14→14
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.202
S = 1.04
4782 reflections
245 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.4138P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Extinction correction: SHELXL (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.060 (11)

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}
O1	0.06071 (19)	0.86788 (15)	0.68377 (15)	0.0598 (5)
O2	−0.1148 (3)	0.8780 (2)	0.5309 (2)	0.0948 (8)
O3	−0.3040 (3)	0.37482 (19)	0.13567 (18)	0.0835 (6)
O4	−0.7070 (2)	0.5897 (2)	0.31738 (19)	0.0879 (7)
C1	−0.2464 (3)	0.5223 (2)	0.3518 (2)	0.0593 (6)
H1	−0.143764	0.504369	0.357291	0.071*
C2	−0.3584 (3)	0.4594 (2)	0.2359 (2)	0.0606 (6)
C3	−0.5109 (3)	0.4842 (2)	0.2268 (2)	0.0630 (7)
H3	−0.585815	0.442242	0.149246	0.076*
C4	−0.5514 (3)	0.5729 (2)	0.3353 (2)	0.0616 (6)
C5	−0.4413 (3)	0.6365 (2)	0.4506 (2)	0.0592 (6)
H5	−0.469808	0.695759	0.522359	0.071*
C6	−0.2869 (3)	0.6112 (2)	0.4585 (2)	0.0536 (6)
C7	−0.1637 (3)	0.6853 (2)	0.5823 (2)	0.0599 (6)
H7A	−0.218876	0.699926	0.654003	0.072*
H7B	−0.088345	0.630395	0.588522	0.072*
C8	−0.0708 (3)	0.8180 (2)	0.59202 (19)	0.0504 (5)
C9	0.1649 (3)	0.9959 (2)	0.7017 (2)	0.0504 (5)
H9	0.143304	1.010726	0.622524	0.060*
C10	0.3389 (3)	0.9848 (2)	0.72620 (19)	0.0503 (5)
C11	0.3878 (3)	0.9112 (3)	0.7918 (3)	0.0698 (7)
H11	0.311265	0.862025	0.818700	0.084*
C12	0.5495 (4)	0.9096 (3)	0.8181 (3)	0.0836 (9)
H12	0.581182	0.860409	0.863666	0.100*
C13	0.6628 (4)	0.9794 (3)	0.7781 (3)	0.0797 (8)
H13	0.771632	0.978449	0.796676	0.096*
C14	0.6161 (4)	1.0504 (3)	0.7110 (3)	0.0831 (9)
H14	0.693159	1.097307	0.682559	0.100*
C15	0.4544 (3)	1.0536 (3)	0.6845 (3)	0.0683 (7)
H15	0.423666	1.102371	0.638211	0.082*
C16	0.1289 (2)	1.1093 (2)	0.8108 (2)	0.0495 (5)
C17	0.1159 (3)	1.1014 (3)	0.9267 (2)	0.0660 (7)
H17	0.129286	1.024538	0.938563	0.079*
C18	0.0833 (4)	1.2066 (3)	1.0257 (3)	0.0804 (8)
H18	0.072381	1.199310	1.102884	0.096*
C19	0.0673 (4)	1.3205 (3)	1.0099 (3)	0.0890 (9)
H19	0.044447	1.391048	1.075939	0.107*
C20	0.0848 (5)	1.3307 (3)	0.8974 (4)	0.1044 (11)
H20	0.076628	1.409502	0.887418	0.125*

C21	0.1145 (4)	1.2251 (3)	0.7976 (3)	0.0816 (8)
H21	0.124898	1.233051	0.720604	0.098*
C22	−0.4026 (5)	0.3230 (4)	0.0098 (3)	0.1043 (11)
H22A	−0.350462	0.265698	−0.050669	0.156*
H22B	−0.506572	0.272258	0.008731	0.156*
H22C	−0.417052	0.396179	−0.013418	0.156*
C23	−0.7547 (4)	0.6812 (3)	0.4234 (3)	0.0870 (9)
H23A	−0.865185	0.683867	0.398647	0.130*
H23B	−0.745738	0.652439	0.493080	0.130*
H23C	−0.685371	0.769232	0.450510	0.130*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0603 (10)	0.0519 (9)	0.0560 (9)	−0.0077 (7)	−0.0144 (7)	0.0265 (7)
O2	0.0892 (14)	0.0892 (14)	0.0945 (14)	−0.0230 (11)	−0.0352 (11)	0.0600 (12)
O3	0.0963 (15)	0.0707 (12)	0.0643 (12)	0.0199 (11)	0.0146 (10)	0.0064 (10)
O4	0.0588 (11)	0.0948 (15)	0.0795 (13)	0.0157 (10)	−0.0064 (9)	0.0086 (11)
C1	0.0568 (14)	0.0500 (13)	0.0629 (15)	0.0052 (11)	0.0025 (11)	0.0198 (11)
C2	0.0688 (16)	0.0474 (13)	0.0523 (13)	0.0033 (11)	0.0076 (11)	0.0113 (11)
C3	0.0616 (15)	0.0540 (14)	0.0518 (13)	−0.0018 (11)	−0.0054 (11)	0.0094 (11)
C4	0.0525 (13)	0.0567 (14)	0.0604 (14)	0.0013 (11)	−0.0010 (11)	0.0156 (12)
C5	0.0613 (14)	0.0504 (13)	0.0503 (13)	0.0010 (11)	0.0037 (11)	0.0106 (10)
C6	0.0553 (13)	0.0443 (12)	0.0510 (12)	−0.0028 (10)	−0.0016 (10)	0.0178 (10)
C7	0.0621 (14)	0.0548 (14)	0.0528 (13)	−0.0013 (11)	−0.0053 (11)	0.0222 (11)
C8	0.0526 (12)	0.0509 (12)	0.0396 (11)	0.0018 (10)	−0.0014 (9)	0.0171 (9)
C9	0.0516 (12)	0.0467 (12)	0.0463 (11)	−0.0011 (9)	−0.0035 (9)	0.0211 (10)
C10	0.0530 (12)	0.0456 (12)	0.0405 (11)	0.0050 (10)	0.0025 (9)	0.0092 (9)
C11	0.0599 (15)	0.0807 (18)	0.0779 (17)	0.0186 (13)	0.0100 (13)	0.0422 (15)
C12	0.0680 (18)	0.100 (2)	0.091 (2)	0.0334 (17)	0.0089 (16)	0.0436 (18)
C13	0.0581 (16)	0.087 (2)	0.0780 (19)	0.0231 (15)	0.0132 (14)	0.0135 (16)
C14	0.0626 (17)	0.090 (2)	0.092 (2)	0.0100 (15)	0.0275 (15)	0.0309 (18)
C15	0.0651 (16)	0.0708 (17)	0.0677 (16)	0.0103 (13)	0.0143 (13)	0.0286 (13)
C16	0.0382 (10)	0.0517 (12)	0.0535 (12)	0.0034 (9)	−0.0027 (9)	0.0223 (10)
C17	0.0748 (17)	0.0646 (16)	0.0555 (14)	0.0150 (13)	0.0068 (12)	0.0235 (12)
C18	0.0821 (19)	0.089 (2)	0.0578 (16)	0.0175 (16)	0.0107 (14)	0.0180 (15)
C19	0.082 (2)	0.076 (2)	0.090 (2)	0.0287 (16)	0.0146 (17)	0.0090 (17)
C20	0.140 (3)	0.076 (2)	0.115 (3)	0.052 (2)	0.036 (2)	0.042 (2)
C21	0.106 (2)	0.0687 (18)	0.0843 (19)	0.0332 (16)	0.0236 (17)	0.0395 (16)
C22	0.130 (3)	0.094 (2)	0.0564 (17)	0.018 (2)	0.0113 (18)	0.0010 (16)
C23	0.0724 (18)	0.089 (2)	0.096 (2)	0.0257 (16)	0.0198 (16)	0.0289 (18)

Geometric parameters (Å, º)

O1—C8	1.317 (2)	C11—H11	0.9300
O1—C9	1.460 (3)	C12—C13	1.359 (4)
O2—C8	1.197 (3)	C12—H12	0.9300
O3—C2	1.372 (3)	C13—C14	1.357 (4)

O3—C22	1.427 (4)	C13—H13	0.9300
O4—C4	1.374 (3)	C14—C15	1.385 (4)
O4—C23	1.416 (3)	C14—H14	0.9300
C1—C6	1.378 (3)	C15—H15	0.9300
C1—C2	1.390 (3)	C16—C21	1.364 (3)
C1—H1	0.9300	C16—C17	1.376 (3)
C2—C3	1.374 (3)	C17—C18	1.384 (4)
C3—C4	1.391 (3)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.360 (4)
C4—C5	1.377 (3)	C18—H18	0.9300
C5—C6	1.392 (3)	C19—C20	1.356 (5)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.504 (3)	C20—C21	1.381 (4)
C7—C8	1.496 (3)	C20—H20	0.9300
C7—H7A	0.9700	C21—H21	0.9300
C7—H7B	0.9700	C22—H22A	0.9600
C9—C16	1.510 (3)	C22—H22B	0.9600
C9—C10	1.511 (3)	C22—H22C	0.9600
C9—H9	0.9800	C23—H23A	0.9600
C10—C11	1.375 (3)	C23—H23B	0.9600
C10—C15	1.378 (3)	C23—H23C	0.9600
C11—C12	1.381 (4)		

C8—O1—C9	117.82 (16)	C13—C12—C11	120.6 (3)
C2—O3—C22	118.2 (2)	C13—C12—H12	119.7
C4—O4—C23	117.6 (2)	C11—C12—H12	119.7
C6—C1—C2	120.2 (2)	C14—C13—C12	119.6 (3)
C6—C1—H1	119.9	C14—C13—H13	120.2
C2—C1—H1	119.9	C12—C13—H13	120.2
O3—C2—C3	124.4 (2)	C13—C14—C15	120.5 (3)
O3—C2—C1	115.1 (2)	C13—C14—H14	119.8
C3—C2—C1	120.5 (2)	C15—C14—H14	119.8
C2—C3—C4	119.0 (2)	C10—C15—C14	120.4 (3)
C2—C3—H3	120.5	C10—C15—H15	119.8
C4—C3—H3	120.5	C14—C15—H15	119.8
O4—C4—C5	124.0 (2)	C21—C16—C17	118.3 (2)
O4—C4—C3	114.8 (2)	C21—C16—C9	120.0 (2)
C5—C4—C3	121.2 (2)	C17—C16—C9	121.6 (2)
C4—C5—C6	119.3 (2)	C16—C17—C18	120.8 (3)
C4—C5—H5	120.3	C16—C17—H17	119.6
C6—C5—H5	120.3	C18—C17—H17	119.6
C1—C6—C5	119.9 (2)	C19—C18—C17	119.9 (3)
C1—C6—C7	120.6 (2)	C19—C18—H18	120.0
C5—C6—C7	119.5 (2)	C17—C18—H18	120.0
C8—C7—C6	112.35 (18)	C20—C19—C18	119.7 (3)
C8—C7—H7A	109.1	C20—C19—H19	120.2
C6—C7—H7A	109.1	C18—C19—H19	120.2
C8—C7—H7B	109.1	C19—C20—C21	120.6 (3)

C6—C7—H7B	109.1	C19—C20—H20	119.7
H7A—C7—H7B	107.9	C21—C20—H20	119.7
O2—C8—O1	122.9 (2)	C16—C21—C20	120.7 (3)
O2—C8—C7	124.7 (2)	C16—C21—H21	119.7
O1—C8—C7	112.15 (18)	C20—C21—H21	119.7
O1—C9—C16	109.94 (18)	O3—C22—H22A	109.5
O1—C9—C10	107.36 (16)	O3—C22—H22B	109.5
C16—C9—C10	112.50 (17)	H22A—C22—H22B	109.5
O1—C9—H9	109.0	O3—C22—H22C	109.5
C16—C9—H9	109.0	H22A—C22—H22C	109.5
C10—C9—H9	109.0	H22B—C22—H22C	109.5
C11—C10—C15	118.3 (2)	O4—C23—H23A	109.5
C11—C10—C9	122.4 (2)	O4—C23—H23B	109.5
C15—C10—C9	119.2 (2)	H23A—C23—H23B	109.5
C10—C11—C12	120.5 (3)	O4—C23—H23C	109.5
C10—C11—H11	119.7	H23A—C23—H23C	109.5
C12—C11—H11	119.7	H23B—C23—H23C	109.5

C22—O3—C2—C3	8.9 (4)	O1—C9—C10—C11	−33.9 (3)
C22—O3—C2—C1	−170.5 (2)	C16—C9—C10—C11	87.2 (3)
C6—C1—C2—O3	178.9 (2)	O1—C9—C10—C15	147.8 (2)
C6—C1—C2—C3	−0.6 (4)	C16—C9—C10—C15	−91.1 (2)
O3—C2—C3—C4	−179.6 (2)	C15—C10—C11—C12	1.8 (4)
C1—C2—C3—C4	−0.1 (4)	C9—C10—C11—C12	−176.5 (2)
C23—O4—C4—C5	1.8 (4)	C10—C11—C12—C13	−0.9 (5)
C23—O4—C4—C3	−178.6 (2)	C11—C12—C13—C14	−0.4 (5)
C2—C3—C4—O4	−179.1 (2)	C12—C13—C14—C15	0.8 (5)
C2—C3—C4—C5	0.5 (4)	C11—C10—C15—C14	−1.4 (4)
O4—C4—C5—C6	179.4 (2)	C9—C10—C15—C14	176.9 (2)
C3—C4—C5—C6	−0.2 (4)	C13—C14—C15—C10	0.1 (4)
C2—C1—C6—C5	0.9 (3)	O1—C9—C16—C21	−135.5 (2)
C2—C1—C6—C7	−176.7 (2)	C10—C9—C16—C21	104.9 (3)
C4—C5—C6—C1	−0.5 (3)	O1—C9—C16—C17	47.0 (3)
C4—C5—C6—C7	177.1 (2)	C10—C9—C16—C17	−72.6 (3)
C1—C6—C7—C8	91.1 (3)	C21—C16—C17—C18	2.3 (4)
C5—C6—C7—C8	−86.6 (3)	C9—C16—C17—C18	179.8 (2)
C9—O1—C8—O2	−6.4 (3)	C16—C17—C18—C19	−1.5 (4)
C9—O1—C8—C7	178.60 (19)	C17—C18—C19—C20	−0.6 (5)
C6—C7—C8—O2	20.2 (4)	C18—C19—C20—C21	1.7 (6)
C6—C7—C8—O1	−164.9 (2)	C17—C16—C21—C20	−1.2 (4)
C8—O1—C9—C16	98.7 (2)	C9—C16—C21—C20	−178.7 (3)
C8—O1—C9—C10	−138.7 (2)	C19—C20—C21—C16	−0.8 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2	0.98	2.30	2.667 (3)	101

C9—H9···O2^{i}	0.98	2.50	3.444 (3)	162

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

Diphenylmethyl 2-(3,4,5-trimethoxyphenyl)acetate (II)

Crystal data

$C_{24}H_{24}O_5$
M_r = 392.43
Monoclinic, $P2_1/n$
a = 17.2290 (14) Å
b = 5.5037 (5) Å
c = 22.1140 (18) Å
β = 92.256 (2)°
V = 2095.3 (3) Å^3
Z = 4
F(000) = 832
D_x = 1.244 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5708 reflections
θ = 2.4–21.2°
μ = 0.09 mm^{-1}
T = 300 K
Block, colourless
0.28 × 0.09 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: i-mu-s microfocus source
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.694, T_{max} = 0.746
39211 measured reflections
5016 independent reflections
2516 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 28.0°, θ_{min} = 1.8°
h = −22→21
k = −7→7
l = −22→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.176
S = 1.00
5016 reflections
263 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0684P)^2 + 0.6429P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: SHELXL (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0182 (19)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.61673 (10)	0.1274 (3)	0.05557 (6)	0.0636 (5)
O2	0.58110 (11)	−0.1961 (3)	0.00128 (7)	0.0774 (5)
O3	0.85376 (10)	0.5998 (4)	−0.03155 (8)	0.0798 (6)
O4	0.82226 (11)	−0.0249 (4)	−0.17236 (8)	0.0859 (6)
O5	0.90848 (10)	0.3195 (4)	−0.11910 (8)	0.0862 (6)
C1	0.72746 (12)	0.4012 (4)	−0.04036 (9)	0.0546 (6)

H1	0.706890	0.501478	−0.011177	0.066*
C2	0.80384 (13)	0.4295 (5)	−0.05603 (10)	0.0565 (6)
C3	0.83399 (13)	0.2815 (5)	−0.10043 (10)	0.0610 (7)
C4	0.78760 (14)	0.1072 (5)	−0.12858 (10)	0.0613 (6)
C5	0.71122 (13)	0.0768 (4)	−0.11256 (9)	0.0575 (6)
H5	0.680153	−0.040984	−0.131508	0.069*
C6	0.68155 (12)	0.2237 (4)	−0.06806 (9)	0.0507 (6)
C7	0.59898 (12)	0.1867 (5)	−0.04865 (9)	0.0554 (6)
H7A	0.577106	0.341746	−0.037250	0.066*
H7B	0.567537	0.122130	−0.082264	0.066*
C8	0.59723 (12)	0.0140 (5)	0.00406 (9)	0.0494 (5)
C9	0.61902 (14)	−0.0116 (4)	0.11119 (9)	0.0580 (6)
H9	0.603757	−0.179139	0.101590	0.070*
C10	0.70113 (14)	−0.0137 (4)	0.13712 (9)	0.0573 (6)
C11	0.75246 (16)	0.1724 (5)	0.12627 (12)	0.0738 (7)
H11	0.736653	0.302650	0.101974	0.089*
C12	0.82733 (18)	0.1664 (6)	0.15134 (14)	0.0893 (9)
H12	0.861775	0.291515	0.143454	0.107*
C13	0.85089 (19)	−0.0237 (7)	0.18780 (14)	0.0899 (10)
H13	0.901014	−0.026577	0.205006	0.108*
C14	0.8005 (2)	−0.2082 (7)	0.19871 (13)	0.0912 (10)
H14	0.816513	−0.336963	0.223414	0.109*
C15	0.72640 (18)	−0.2053 (5)	0.17351 (12)	0.0768 (8)
H15	0.692821	−0.333234	0.180921	0.092*
C16	0.56005 (13)	0.0950 (4)	0.15319 (9)	0.0559 (6)
C17	0.54475 (15)	−0.0247 (5)	0.20629 (11)	0.0732 (7)
H17	0.571537	−0.166755	0.216249	0.088*
C18	0.49038 (16)	0.0633 (6)	0.24472 (12)	0.0839 (9)
H18	0.480967	−0.019706	0.280326	0.101*
C19	0.45026 (16)	0.2707 (6)	0.23110 (13)	0.0812 (8)
H19	0.413734	0.330233	0.257196	0.097*
C20	0.46445 (17)	0.3897 (6)	0.17866 (14)	0.0851 (8)
H20	0.436827	0.530448	0.168889	0.102*
C21	0.51904 (16)	0.3054 (5)	0.13979 (12)	0.0711 (7)
H21	0.528292	0.390302	0.104434	0.085*
C22	0.82561 (16)	0.7587 (5)	0.01338 (12)	0.0789 (8)
H22A	0.866226	0.868081	0.026580	0.118*
H22B	0.782408	0.850000	−0.003331	0.118*
H22C	0.809195	0.665036	0.047205	0.118*
C23	0.78071 (19)	−0.2196 (5)	−0.19993 (13)	0.0898 (9)
H23A	0.812069	−0.295090	−0.229561	0.135*
H23B	0.768119	−0.336789	−0.169695	0.135*
H23C	0.733721	−0.159175	−0.219272	0.135*
C24	0.96593 (19)	0.1834 (11)	−0.08755 (19)	0.179 (2)
H24A	1.015823	0.219968	−0.103154	0.268*
H24B	0.966039	0.224012	−0.045331	0.268*
H24C	0.955212	0.013311	−0.092616	0.268*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0941 (12)	0.0551 (10)	0.0410 (8)	−0.0129 (9)	−0.0040 (8)	0.0041 (7)
O2	0.1106 (14)	0.0619 (12)	0.0595 (10)	−0.0110 (11)	−0.0007 (9)	−0.0093 (9)
O3	0.0633 (11)	0.0989 (14)	0.0781 (12)	−0.0191 (10)	0.0144 (9)	−0.0194 (11)
O4	0.0838 (12)	0.1052 (15)	0.0708 (11)	−0.0005 (11)	0.0304 (9)	−0.0254 (11)
O5	0.0574 (10)	0.1270 (17)	0.0761 (12)	−0.0066 (11)	0.0265 (9)	−0.0072 (11)
C1	0.0535 (13)	0.0660 (15)	0.0450 (12)	0.0037 (12)	0.0079 (10)	0.0004 (11)
C2	0.0489 (13)	0.0717 (16)	0.0492 (12)	−0.0056 (12)	0.0053 (10)	0.0017 (12)
C3	0.0485 (13)	0.0861 (18)	0.0494 (13)	0.0002 (13)	0.0144 (10)	0.0036 (13)
C4	0.0641 (15)	0.0761 (17)	0.0447 (12)	0.0082 (13)	0.0145 (11)	−0.0032 (12)
C5	0.0586 (14)	0.0704 (16)	0.0439 (12)	−0.0009 (12)	0.0068 (10)	−0.0011 (11)
C6	0.0466 (12)	0.0655 (15)	0.0402 (11)	0.0031 (11)	0.0045 (9)	0.0066 (11)
C7	0.0457 (12)	0.0795 (16)	0.0409 (11)	0.0010 (11)	0.0004 (9)	0.0031 (11)
C8	0.0405 (11)	0.0641 (16)	0.0441 (12)	0.0016 (11)	0.0061 (9)	−0.0060 (12)
C9	0.0848 (17)	0.0471 (13)	0.0419 (12)	−0.0093 (12)	0.0001 (11)	0.0049 (10)
C10	0.0752 (16)	0.0541 (14)	0.0428 (12)	0.0080 (13)	0.0068 (11)	−0.0048 (11)
C11	0.0811 (19)	0.0673 (18)	0.0720 (17)	0.0013 (15)	−0.0073 (14)	0.0010 (14)
C12	0.078 (2)	0.093 (2)	0.096 (2)	0.0014 (17)	−0.0086 (17)	−0.0139 (19)
C13	0.079 (2)	0.113 (3)	0.0759 (19)	0.034 (2)	−0.0136 (16)	−0.029 (2)
C14	0.101 (2)	0.101 (3)	0.0714 (18)	0.041 (2)	−0.0015 (17)	0.0027 (18)
C15	0.095 (2)	0.0737 (19)	0.0624 (15)	0.0222 (16)	0.0108 (15)	0.0083 (14)
C16	0.0619 (14)	0.0592 (15)	0.0461 (12)	−0.0111 (12)	−0.0039 (10)	0.0006 (11)
C17	0.0686 (16)	0.0880 (19)	0.0632 (15)	−0.0053 (15)	0.0052 (13)	0.0181 (15)
C18	0.0687 (17)	0.119 (3)	0.0645 (17)	−0.0058 (18)	0.0144 (14)	0.0183 (17)
C19	0.0638 (17)	0.107 (2)	0.0728 (18)	−0.0014 (17)	0.0071 (14)	−0.0101 (18)
C20	0.085 (2)	0.089 (2)	0.082 (2)	0.0120 (17)	0.0052 (16)	−0.0068 (17)
C21	0.0866 (18)	0.0663 (17)	0.0603 (15)	−0.0007 (15)	0.0017 (14)	0.0045 (13)
C22	0.0846 (18)	0.085 (2)	0.0675 (16)	−0.0140 (16)	0.0031 (14)	−0.0134 (15)
C23	0.121 (2)	0.080 (2)	0.0706 (17)	0.0092 (19)	0.0276 (17)	−0.0136 (16)
C24	0.060 (2)	0.334 (7)	0.144 (4)	0.053 (3)	0.020 (2)	0.058 (4)

Geometric parameters (Å, º)

O1—C8	1.330 (3)	C12—C13	1.372 (4)
O1—C9	1.448 (2)	C12—H12	0.9300
O2—C8	1.191 (3)	C13—C14	1.363 (4)
O3—C2	1.369 (3)	C13—H13	0.9300
O3—C22	1.423 (3)	C14—C15	1.373 (4)
O4—C4	1.367 (3)	C14—H14	0.9300
O4—C23	1.414 (3)	C15—H15	0.9300
O5—C3	1.379 (3)	C16—C21	1.382 (3)
O5—C24	1.405 (4)	C16—C17	1.381 (3)
C1—C2	1.383 (3)	C17—C18	1.377 (4)
C1—C6	1.384 (3)	C17—H17	0.9300
C1—H1	0.9300	C18—C19	1.362 (4)
C2—C3	1.392 (3)	C18—H18	0.9300

C3—C4	1.381 (3)	C19—C20	1.362 (4)
C4—C5	1.386 (3)	C19—H19	0.9300
C5—C6	1.387 (3)	C20—C21	1.380 (4)
C5—H5	0.9300	C20—H20	0.9300
C6—C7	1.516 (3)	C21—H21	0.9300
C7—C8	1.505 (3)	C22—H22A	0.9600
C7—H7A	0.9700	C22—H22B	0.9600
C7—H7B	0.9700	C22—H22C	0.9600
C9—C10	1.506 (3)	C23—H23A	0.9600
C9—C16	1.521 (3)	C23—H23B	0.9600
C9—H9	0.9800	C23—H23C	0.9600
C10—C11	1.381 (4)	C24—H24A	0.9600
C10—C15	1.386 (3)	C24—H24B	0.9600
C11—C12	1.384 (4)	C24—H24C	0.9600
C11—H11	0.9300		

C8—O1—C9	118.49 (18)	C14—C13—C12	119.7 (3)
C2—O3—C22	118.07 (19)	C14—C13—H13	120.1
C4—O4—C23	118.7 (2)	C12—C13—H13	120.1
C3—O5—C24	114.6 (2)	C13—C14—C15	120.5 (3)
C2—C1—C6	120.1 (2)	C13—C14—H14	119.7
C2—C1—H1	119.9	C15—C14—H14	119.7
C6—C1—H1	119.9	C14—C15—C10	120.7 (3)
O3—C2—C1	124.6 (2)	C14—C15—H15	119.7
O3—C2—C3	115.68 (19)	C10—C15—H15	119.7
C1—C2—C3	119.7 (2)	C21—C16—C17	118.0 (2)
C4—C3—O5	119.9 (2)	C21—C16—C9	122.7 (2)
C4—C3—C2	119.9 (2)	C17—C16—C9	119.3 (2)
O5—C3—C2	120.0 (2)	C18—C17—C16	120.9 (3)
O4—C4—C3	115.3 (2)	C18—C17—H17	119.5
O4—C4—C5	124.2 (2)	C16—C17—H17	119.5
C3—C4—C5	120.5 (2)	C19—C18—C17	120.6 (3)
C4—C5—C6	119.4 (2)	C19—C18—H18	119.7
C4—C5—H5	120.3	C17—C18—H18	119.7
C6—C5—H5	120.3	C20—C19—C18	119.0 (3)
C1—C6—C5	120.3 (2)	C20—C19—H19	120.5
C1—C6—C7	119.7 (2)	C18—C19—H19	120.5
C5—C6—C7	119.9 (2)	C19—C20—C21	121.2 (3)
C8—C7—C6	110.59 (17)	C19—C20—H20	119.4
C8—C7—H7A	109.5	C21—C20—H20	119.4
C6—C7—H7A	109.5	C20—C21—C16	120.2 (3)
C8—C7—H7B	109.5	C20—C21—H21	119.9
C6—C7—H7B	109.5	C16—C21—H21	119.9
H7A—C7—H7B	108.1	O3—C22—H22A	109.5
O2—C8—O1	123.4 (2)	O3—C22—H22B	109.5
O2—C8—C7	125.8 (2)	H22A—C22—H22B	109.5
O1—C8—C7	110.8 (2)	O3—C22—H22C	109.5
O1—C9—C10	108.75 (18)	H22A—C22—H22C	109.5

O1—C9—C16	108.58 (19)	H22B—C22—H22C	109.5
C10—C9—C16	114.24 (17)	O4—C23—H23A	109.5
O1—C9—H9	108.4	O4—C23—H23B	109.5
C10—C9—H9	108.4	H23A—C23—H23B	109.5
C16—C9—H9	108.4	O4—C23—H23C	109.5
C11—C10—C15	118.5 (2)	H23A—C23—H23C	109.5
C11—C10—C9	121.8 (2)	H23B—C23—H23C	109.5
C15—C10—C9	119.7 (2)	O5—C24—H24A	109.5
C10—C11—C12	120.4 (3)	O5—C24—H24B	109.5
C10—C11—H11	119.8	H24A—C24—H24B	109.5
C12—C11—H11	119.8	O5—C24—H24C	109.5
C13—C12—C11	120.2 (3)	H24A—C24—H24C	109.5
C13—C12—H12	119.9	H24B—C24—H24C	109.5
C11—C12—H12	119.9		

C22—O3—C2—C1	0.3 (3)	C6—C7—C8—O1	79.9 (2)
C22—O3—C2—C3	179.0 (2)	C8—O1—C9—C10	116.5 (2)
C6—C1—C2—O3	179.7 (2)	C8—O1—C9—C16	−118.7 (2)
C6—C1—C2—C3	1.0 (3)	O1—C9—C10—C11	27.6 (3)
C24—O5—C3—C4	−92.2 (4)	C16—C9—C10—C11	−93.8 (3)
C24—O5—C3—C2	92.1 (4)	O1—C9—C10—C15	−153.1 (2)
O3—C2—C3—C4	−178.8 (2)	C16—C9—C10—C15	85.5 (3)
C1—C2—C3—C4	0.0 (4)	C15—C10—C11—C12	0.0 (4)
O3—C2—C3—O5	−3.1 (3)	C9—C10—C11—C12	179.3 (2)
C1—C2—C3—O5	175.7 (2)	C10—C11—C12—C13	−0.7 (4)
C23—O4—C4—C3	175.0 (2)	C11—C12—C13—C14	0.8 (4)
C23—O4—C4—C5	−5.7 (4)	C12—C13—C14—C15	0.0 (5)
O5—C3—C4—O4	2.9 (3)	C13—C14—C15—C10	−0.8 (4)
C2—C3—C4—O4	178.7 (2)	C11—C10—C15—C14	0.8 (4)
O5—C3—C4—C5	−176.3 (2)	C9—C10—C15—C14	−178.5 (2)
C2—C3—C4—C5	−0.6 (4)	O1—C9—C16—C21	−6.0 (3)
O4—C4—C5—C6	−179.0 (2)	C10—C9—C16—C21	115.6 (2)
C3—C4—C5—C6	0.2 (3)	O1—C9—C16—C17	172.25 (19)
C2—C1—C6—C5	−1.4 (3)	C10—C9—C16—C17	−66.2 (3)
C2—C1—C6—C7	177.4 (2)	C21—C16—C17—C18	−0.1 (4)
C4—C5—C6—C1	0.8 (3)	C9—C16—C17—C18	−178.4 (2)
C4—C5—C6—C7	−178.0 (2)	C16—C17—C18—C19	0.1 (4)
C1—C6—C7—C8	−87.0 (3)	C17—C18—C19—C20	0.3 (4)
C5—C6—C7—C8	91.8 (2)	C18—C19—C20—C21	−0.7 (4)
C9—O1—C8—O2	0.4 (3)	C19—C20—C21—C16	0.7 (4)
C9—O1—C8—C7	−179.34 (18)	C17—C16—C21—C20	−0.3 (4)
C6—C7—C8—O2	−99.8 (3)	C9—C16—C21—C20	177.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2	0.98	2.24	2.691 (3)	107

C21—H21···O1	0.93	2.39	2.740 (3)	102
C19—H19···O4^{i}	0.93	2.50	3.427 (3)	175

Symmetry code: (i) $x-1/2, -y+1/2, z+1/2$.