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Crystal structure of 5-[(4-carboxybenzyl)oxy]- isophthalic acid

Md. Serajul Haque Faizi,^a Musheer Ahmad,^b Akram Ali^c and Vadim A. Potaskalov^{d*}

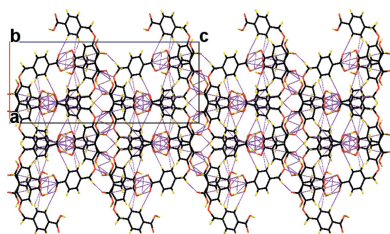
^aDepartment of Chemistry, College of Science, Sultan Qaboos University, PO Box, 36 Al-Khod 123, Muscat, Sultanate of Oman, ^bDepartment of Applied Chemistry, Aligarh Muslim University, 202 002 UP, India, ^cNational Taras Shevchenko University, Department of Chemistry, Volodymyrska str. 64, 01601 Kyiv, Ukraine, and ^dDepartment of General and Inorganic Chemistry, National Technical University of Ukraine, Kyiv Polytechnic Institute, 37 Prospect Peremogy, 03056 Kiev, Ukraine. *Correspondence e-mail: potaskalov@xtf.kpi.ua

The molecular shape of the title compound, C₁₆H₁₂O₇, is bent around the central CH₂–O bond. The two benzene rings are almost perpendicular to one another, making a dihedral angle of 87.78 (7)°. In the crystal, each molecule is linked to three others by three pairs of O–H···O hydrogen bonds, forming undulating sheets parallel to the *bc* plane and enclosing R₂²(8) ring motifs. The sheets are linked by C–H···O hydrogen bonds and C–H···π interactions, forming a three-dimensional network.

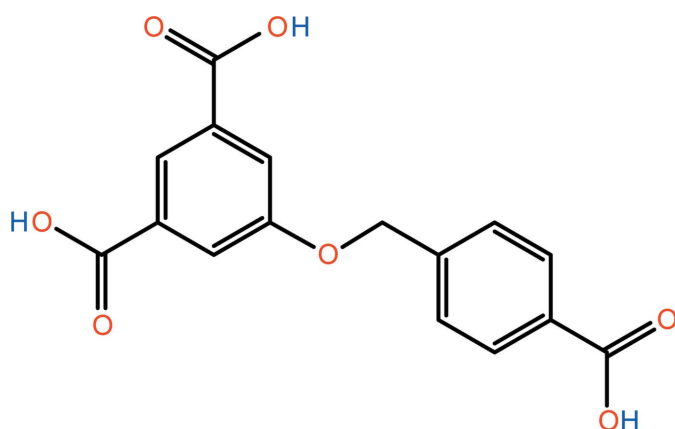
1. Chemical context

The design and synthesis of coordination polymers continues to attract interest due to their architectures as well as their potential applications (Erxleben, 2003). Recently, the rational design and synthesis of novel coordination polymers have attracted intense attention in the field of supramolecular chemistry and crystal engineering (Zhang *et al.*, 2011). To date, large numbers of coordination architectures with interesting compositions and properties have been prepared using a wide variety of aromatic polycarboxylate-based ligands (Cambridge Structural Database; Groom *et al.*, 2016). The title compound (CIA), a tricarboxylate ligand, has been shown to be a good candidate for the construction of coordination polymers (Ahmad *et al.*, 2012*a,b*). Tricarboxylate ligands have been used in the synthesis of metal-organic framework complexes (MOFs) because of their photoelectric properties and for their potential nitrobenzene sensing (Hou *et al.*, 2016). A Cd^{II} MOF based on CIA has been structurally and functionally characterized, and was shown to be a highly selective CH₂Cl₂ fluorescent sensor (Xia *et al.*, 2015). A series of one-, two- and three-dimensional coordination polymers based on CIA have been structurally characterized and shown to display photoluminescence (Liu *et al.*, 2012).

We have crystallized a reported polycarboxylate containing the ligand, 5-[(4-carboxybenzyl)oxy]isophthalic acid (CIA), which has the advantage of being flexible and has conformational freedom allowing it to conform to the coordination environment of transition metal ions. We report herein on the crystal structure of the title tricarboxylate ligand (CIA), synthesized by a reported procedure (Ahmad *et al.*, 2012*a,b*).



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2. Structural commentary

The molecular structure of the title compound (CIA) is illustrated in Fig. 1. The bond lengths and bond angles are normal and close to the values observed in related structures (Li & Ma 2011; He *et al.*, 2014). The molecular shape of the title compound is bent around the central C9—O5 bond; the spacer ether group exhibits a C10—C9—O5—C1 torsion angle of $-84.35(19)^\circ$. The benzene rings, C1—C6 and C10—C15, are roughly perpendicular to each another, with a dihedral angle of $87.78(7)^\circ$. The three O=C—O bond angles of the carboxylic acid groups are $123.17(17)$, $123.62(17)$, $123.74(17)^\circ$, respectively, for O1=C7—O2, O3=C8—O4 and O6=C16—O7.

3. Supramolecular features

In the crystal, each molecule is linked to three others by three pairs of O—H...O hydrogen bonds, forming undulating sheets parallel to the *bc* plane and enclosing $R_2^2(8)$ ring motifs (Table 1 and Fig. 2). The sheets are linked by C—H...O

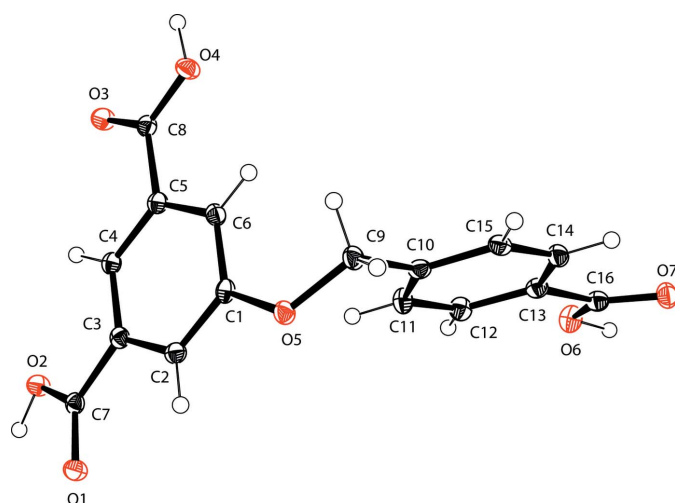


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 40% probability level.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

Cg2 is the centroid of the C10—C15 ring.

<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>
O2—H2A...O1 ⁱ	0.95 (3)	1.70 (3)	2.6426 (19)	176 (2)
O4—H4A...O7 ⁱⁱ	0.99 (3)	1.62 (3)	2.6086 (19)	175 (3)
O6—H6A...O3 ⁱⁱⁱ	0.93 (3)	1.72 (3)	2.6486 (19)	179 (4)
C9—H9A...O1 ^{iv}	0.97	2.51	3.272 (2)	135
C11—H11A...O3 ^v	0.93	2.45	3.170 (2)	135
C14—H14A...O4 ^{vi}	0.93	2.56	3.245 (2)	131
C9—H9B...Cg2 ^{vii}	0.97	2.97	3.779 (2)	141

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $x+\frac{1}{2}, y+1, -z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, y-1, -z+\frac{1}{2}$; (iv) $-x+1, -y, -z$; (v) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (vi) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (vii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.

hydrogen bonds and C—H... π interactions, forming a three-dimensional network (Table 1 and Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (Version 5.37, update February 2016; Groom *et al.*, 2016) for the title compound gave 42 hits. The majority of these compounds are coordination polymers involving a secondary ligand. Ten structures concern coordination polymers of the title ligand itself. For example, *catena*-[μ_6 -5-(4-carboxybenzyloxy)-isophthalato-(μ_2 -aqua)barium(II)] where only two of the carboxylic acid groups of the CIA molecule are deprotonated (BEDJOL; Li & Ma, 2012), and *catena*-[bis{ μ_6 -5-[(4-carboxybenzyloxy)isophthalato]}(μ_2 -aqua)tricadmium trihydrate] (IZEBEV; Zhang *et al.*, 2011) where all three carboxylic acid groups of the CIA molecule are deprotonated.

5. Synthesis and crystallization

The starting compound diethyl 5-(4-methoxycarbonylbenzyloxy)isophthalate (DMBI) was prepared by the following

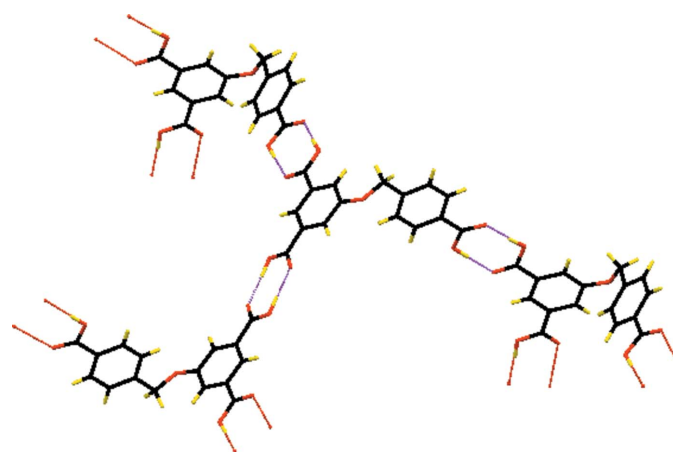


Figure 2
A partial view of the O—H...O hydrogen-bonding interactions between the donor and acceptor oxygen atoms of the carboxylic groups in the crystal of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1 for details).

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₆ H ₁₂ O ₇
<i>M_r</i>	316.26
Crystal system, space group	Orthorhombic, <i>Pbca</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.998 (2), 9.2760 (17), 25.661 (5)
<i>V</i> (Å ³)	2618.0 (8)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
<i>μ</i> (mm ⁻¹)	0.13
Crystal size (mm)	0.27 × 0.21 × 0.16
Data collection	
Diffractometer	Bruker SMART APEX
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2003)
<i>T_{min}</i> , <i>T_{max}</i>	0.966, 0.980
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	12591, 2292, 1912
<i>R_{int}</i>	0.043
(sin θ/λ) _{max} (Å ⁻¹)	0.595
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.040, 0.102, 1.07
No. of reflections	2292
No. of parameters	220
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.25, -0.24

Computer programs: *SMART* and *SAINT* (Bruker, 2003), *SIR97* (Altomare *et al.*, 1999), *DIAMOND* (Brandenburg & Putz, 2006), *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

procedure: 5-hydroxyisophthalic acid diethyl ester (2 g, 8.4 mmol) and dry K₂CO₃ (1.7g, 12.6 mmol) were mixed in dry acetonitrile (10 ml) and stirred for 30 min at 353 K. Then 4-bromomethyl benzoic acid methyl ester (1.9 g, 8.40 mmol)

was added and the resulting solution was refluxed for 24 h. The solution was pored into ice-cold water and the solid precipitate obtained was filtered and dried in air (yield: 2.8 g, 86%). The title compound (CIA) was prepared as follows: DMBI (2 g, 5.17 mmol) was hydrolyzed by refluxing it with 6*N* NaOH solution (20 ml) for 24 h. After cooling to 278 K, the resulting solution was acidified with 6*N* HCl solution to obtain a white precipitate. This was collected by filtration, washed thoroughly with water, and dried in air. The solid powder was dissolved in dimethyl formamide and needle-like crystals were obtained by slow diffusion of diethyl ether into the solution, after 2–3 days (yield: 1.3 g, 80%).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The OH H atoms were located in a difference Fourier map and freely refined. The C-bound H atoms were positioned geometrically and refined using a riding model: C–H = 0.93–0.97 Å with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Acknowledgements

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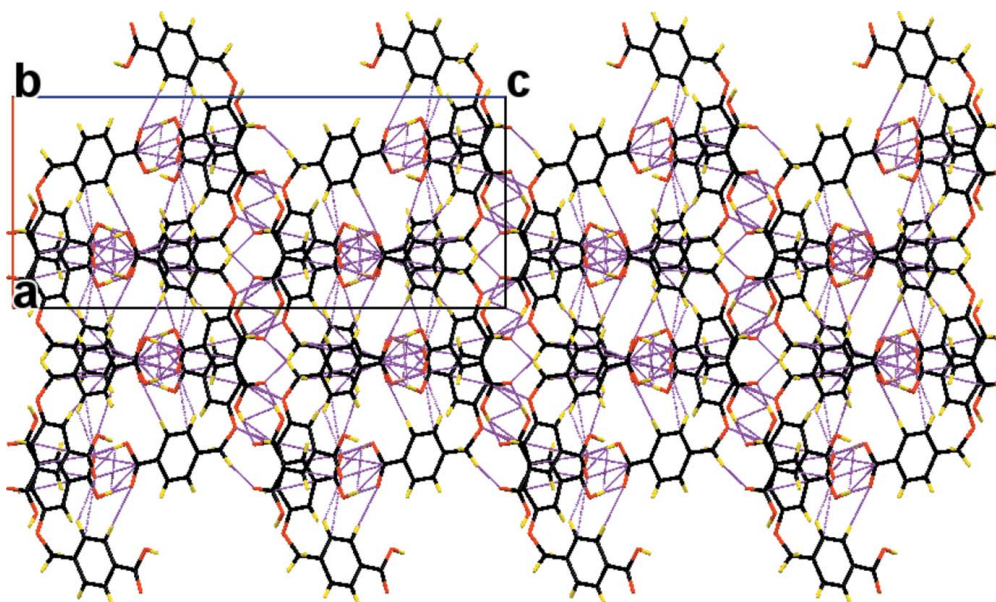


Figure 3

A view along the *b* axis of the crystal packing of the title compound. The O–H···O and C–H···O hydrogen bonds and C–H···π interactions are shown as dashed lines (see Table 1 for details). **Fig 3 hard to make out, too many molecules shown**

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supporting information

Acta Cryst. (2016). E72, 1219-1222 [https://doi.org/10.1107/S2056989016011762]

Crystal structure of 5-[(4-carboxybenzyl)oxy]isophthalic acid

Md. Serajul Haque Faizi, Musheer Ahmad, Akram Ali and Vadim A. Potaskalov

Computing details

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINTE* (Bruker, 2003); data reduction: *SAINTE* (Bruker, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

5-[(4-Carboxybenzyl)oxy]benzene-1,3-dicarboxylic acid

Crystal data

$C_{16}H_{12}O_7$

$M_r = 316.26$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 10.998$ (2) Å

$b = 9.2760$ (17) Å

$c = 25.661$ (5) Å

$V = 2618.0$ (8) Å³

$Z = 8$

$F(000) = 1312$

$D_x = 1.605$ Mg m⁻³

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

Cell parameters from 999 reflections

$\theta = 2.2$ – 25.5°

$\mu = 0.13$ mm⁻¹

$T = 100$ K

Needle, colourless

$0.27 \times 0.21 \times 0.16$ mm

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

/w-scans

Absorption correction: multi-scan
(SADABS; Bruker, 2003)

$T_{\min} = 0.966$, $T_{\max} = 0.980$

12591 measured reflections

2292 independent reflections

1912 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.4^\circ$

$h = -13 \rightarrow 12$

$k = -11 \rightarrow 10$

$l = -30 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.102$

$S = 1.07$

2292 reflections

220 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 atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 1.0476P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.25$ e Å⁻³

$\Delta\rho_{\min} = -0.24$ 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. 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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.54437 (16)	0.2010 (2)	0.06349 (7)	0.0163 (4)
C2	0.64357 (16)	0.1415 (2)	0.03776 (7)	0.0169 (4)
H2	0.6318	0.0727	0.0119	0.020*
C3	0.76100 (16)	0.1855 (2)	0.05087 (7)	0.0158 (4)
C4	0.77916 (16)	0.2916 (2)	0.08860 (7)	0.0162 (4)
H4	0.8574	0.3207	0.0974	0.019*
C5	0.67901 (17)	0.35318 (19)	0.11272 (7)	0.0168 (4)
C6	0.56157 (16)	0.3076 (2)	0.10094 (7)	0.0169 (4)
H6	0.4952	0.3480	0.1179	0.020*
C7	0.86620 (16)	0.1109 (2)	0.02637 (7)	0.0161 (4)
C8	0.70035 (16)	0.4673 (2)	0.15257 (7)	0.0165 (4)
C9	0.32778 (16)	0.1744 (2)	0.08031 (7)	0.0176 (4)
H9A	0.2559	0.1698	0.0585	0.021*
H9B	0.3330	0.2712	0.0944	0.021*
C10	0.31395 (16)	0.0687 (2)	0.12475 (7)	0.0169 (4)
C11	0.41173 (17)	-0.0068 (2)	0.14518 (7)	0.0206 (4)
H11A	0.4889	0.0072	0.1313	0.025*
C12	0.39619 (17)	-0.1030 (2)	0.18599 (7)	0.0205 (4)
H12	0.4629	-0.1514	0.1998	0.025*
C13	0.28067 (17)	-0.1271 (2)	0.20631 (7)	0.0178 (4)
C14	0.18210 (17)	-0.0509 (2)	0.18628 (7)	0.0188 (4)
H14A	0.1048	-0.0654	0.2000	0.023*
C15	0.19867 (16)	0.0462 (2)	0.14616 (7)	0.0169 (4)
H15	0.1324	0.0972	0.1332	0.020*
C16	0.25906 (17)	-0.2367 (2)	0.24740 (7)	0.0187 (4)
O1	0.85402 (11)	0.02572 (14)	-0.00993 (5)	0.0198 (3)
O2	0.97202 (12)	0.14066 (14)	0.04773 (5)	0.0195 (3)
O3	0.80429 (11)	0.49920 (14)	0.16624 (5)	0.0214 (3)
O4	0.60297 (11)	0.52892 (14)	0.17105 (5)	0.0209 (3)
O5	0.43311 (11)	0.14724 (14)	0.04881 (5)	0.0183 (3)
O6	0.35857 (12)	-0.28772 (15)	0.26911 (5)	0.0240 (3)
O7	0.15576 (12)	-0.27618 (14)	0.25925 (5)	0.0235 (3)
H4A	0.627 (3)	0.600 (4)	0.1980 (12)	0.084 (11)*
H6A	0.339 (3)	-0.362 (3)	0.2920 (11)	0.065 (9)*
H2A	1.032 (3)	0.079 (3)	0.0334 (11)	0.067 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0158 (9)	0.0172 (10)	0.0160 (9)	-0.0019 (8)	-0.0005 (7)	0.0044 (7)
C2	0.0213 (10)	0.0149 (10)	0.0145 (9)	-0.0002 (8)	0.0001 (8)	0.0011 (7)
C3	0.0175 (9)	0.0159 (9)	0.0141 (9)	0.0003 (7)	0.0005 (7)	0.0030 (7)
C4	0.0147 (9)	0.0166 (10)	0.0172 (9)	-0.0010 (8)	-0.0009 (7)	0.0021 (7)
C5	0.0212 (10)	0.0148 (9)	0.0144 (9)	0.0006 (8)	0.0009 (8)	0.0037 (7)
C6	0.0165 (9)	0.0174 (10)	0.0168 (9)	0.0012 (8)	0.0024 (7)	0.0022 (7)
C7	0.0182 (10)	0.0163 (10)	0.0138 (9)	-0.0012 (8)	0.0004 (7)	0.0030 (7)
C8	0.0163 (10)	0.0161 (10)	0.0172 (9)	-0.0005 (8)	0.0003 (8)	0.0017 (7)
C9	0.0134 (9)	0.0205 (10)	0.0191 (10)	-0.0011 (8)	0.0010 (8)	-0.0008 (8)
C10	0.0181 (9)	0.0160 (10)	0.0165 (10)	-0.0008 (7)	-0.0009 (7)	-0.0041 (7)
C11	0.0151 (9)	0.0234 (11)	0.0232 (11)	-0.0020 (8)	0.0015 (8)	0.0025 (8)
C12	0.0176 (10)	0.0216 (10)	0.0222 (10)	0.0009 (8)	-0.0014 (8)	0.0009 (8)
C13	0.0193 (10)	0.0171 (10)	0.0169 (10)	-0.0007 (8)	-0.0008 (8)	-0.0022 (7)
C14	0.0154 (9)	0.0215 (10)	0.0194 (10)	-0.0016 (8)	0.0014 (8)	-0.0029 (8)
C15	0.0154 (9)	0.0188 (10)	0.0166 (10)	0.0014 (8)	-0.0007 (7)	-0.0037 (8)
C16	0.0204 (10)	0.0183 (10)	0.0173 (10)	0.0000 (8)	-0.0003 (8)	-0.0020 (8)
O1	0.0183 (7)	0.0211 (7)	0.0199 (7)	0.0009 (6)	0.0004 (5)	-0.0040 (6)
O2	0.0157 (7)	0.0219 (8)	0.0208 (7)	0.0008 (6)	-0.0011 (6)	-0.0037 (6)
O3	0.0161 (7)	0.0241 (8)	0.0240 (8)	-0.0006 (6)	-0.0014 (6)	-0.0058 (6)
O4	0.0151 (7)	0.0231 (8)	0.0245 (8)	0.0009 (6)	0.0010 (6)	-0.0073 (6)
O5	0.0145 (7)	0.0217 (7)	0.0186 (7)	-0.0023 (5)	0.0009 (5)	-0.0023 (5)
O6	0.0233 (8)	0.0250 (8)	0.0238 (8)	-0.0012 (6)	-0.0035 (6)	0.0072 (6)
O7	0.0204 (7)	0.0230 (7)	0.0270 (8)	-0.0007 (6)	0.0057 (6)	0.0041 (6)

Geometric parameters (Å, °)

C1—O5	1.374 (2)	C9—H9A	0.9700
C1—C2	1.389 (3)	C9—H9B	0.9700
C1—C6	1.392 (3)	C10—C11	1.386 (3)
C2—C3	1.396 (3)	C10—C15	1.397 (3)
C2—H2	0.9300	C11—C12	1.387 (3)
C3—C4	1.395 (3)	C11—H11A	0.9300
C3—C7	1.488 (3)	C12—C13	1.391 (3)
C4—C5	1.387 (3)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.393 (3)
C5—C6	1.392 (3)	C13—C16	1.484 (3)
C5—C8	1.490 (3)	C14—C15	1.380 (3)
C6—H6	0.9300	C14—H14A	0.9300
C7—O1	1.229 (2)	C15—H15	0.9300
C7—O2	1.316 (2)	C16—O7	1.232 (2)
C8—O3	1.232 (2)	C16—O6	1.316 (2)
C8—O4	1.303 (2)	O2—H2A	0.95 (3)
C9—O5	1.435 (2)	O4—H4A	0.99 (3)
C9—C10	1.512 (3)	O6—H6A	0.93 (3)

O5—C1—C2	115.15 (16)	C10—C9—H9B	109.0
O5—C1—C6	124.63 (16)	H9A—C9—H9B	107.8
C2—C1—C6	120.22 (17)	C11—C10—C15	118.67 (17)
C1—C2—C3	119.74 (17)	C11—C10—C9	122.34 (16)
C1—C2—H2	120.1	C15—C10—C9	118.99 (16)
C3—C2—H2	120.1	C10—C11—C12	121.00 (17)
C4—C3—C2	120.40 (17)	C10—C11—H11A	119.5
C4—C3—C7	120.68 (16)	C12—C11—H11A	119.5
C2—C3—C7	118.81 (16)	C11—C12—C13	119.93 (17)
C5—C4—C3	119.12 (17)	C11—C12—H12	120.0
C5—C4—H4	120.4	C13—C12—H12	120.0
C3—C4—H4	120.4	C12—C13—C14	119.39 (17)
C4—C5—C6	120.98 (17)	C12—C13—C16	121.51 (17)
C4—C5—C8	118.28 (16)	C14—C13—C16	119.05 (17)
C6—C5—C8	120.73 (16)	C15—C14—C13	120.27 (17)
C1—C6—C5	119.47 (17)	C15—C14—H14A	119.9
C1—C6—H6	120.3	C13—C14—H14A	119.9
C5—C6—H6	120.3	C14—C15—C10	120.70 (17)
O1—C7—O2	123.17 (17)	C14—C15—H15	119.6
O1—C7—C3	122.32 (16)	C10—C15—H15	119.6
O2—C7—C3	114.48 (15)	O7—C16—O6	123.74 (17)
O3—C8—O4	123.62 (17)	O7—C16—C13	121.80 (17)
O3—C8—C5	120.81 (16)	O6—C16—C13	114.45 (16)
O4—C8—C5	115.58 (15)	C7—O2—H2A	109.3 (17)
O5—C9—C10	113.10 (15)	C8—O4—H4A	109.0 (18)
O5—C9—H9A	109.0	C1—O5—C9	120.05 (14)
C10—C9—H9A	109.0	C16—O6—H6A	109.8 (17)
O5—C9—H9B	109.0		
O5—C1—C2—C3	-178.10 (15)	O5—C9—C10—C11	23.7 (2)
C6—C1—C2—C3	2.2 (3)	O5—C9—C10—C15	-156.45 (15)
C1—C2—C3—C4	-1.8 (3)	C15—C10—C11—C12	0.1 (3)
C1—C2—C3—C7	174.41 (16)	C9—C10—C11—C12	179.95 (17)
C2—C3—C4—C5	-0.3 (3)	C10—C11—C12—C13	1.4 (3)
C7—C3—C4—C5	-176.39 (16)	C11—C12—C13—C14	-1.8 (3)
C3—C4—C5—C6	1.9 (3)	C11—C12—C13—C16	175.62 (17)
C3—C4—C5—C8	-179.46 (16)	C12—C13—C14—C15	0.9 (3)
O5—C1—C6—C5	179.77 (16)	C16—C13—C14—C15	-176.60 (16)
C2—C1—C6—C5	-0.6 (3)	C13—C14—C15—C10	0.5 (3)
C4—C5—C6—C1	-1.5 (3)	C11—C10—C15—C14	-1.0 (3)
C8—C5—C6—C1	179.90 (16)	C9—C10—C15—C14	179.12 (17)
C4—C3—C7—O1	-173.84 (17)	C12—C13—C16—O7	-167.37 (18)
C2—C3—C7—O1	10.0 (3)	C14—C13—C16—O7	10.1 (3)
C4—C3—C7—O2	8.0 (2)	C12—C13—C16—O6	11.9 (3)
C2—C3—C7—O2	-168.23 (16)	C14—C13—C16—O6	-170.61 (16)
C4—C5—C8—O3	-4.8 (3)	C2—C1—O5—C9	165.51 (15)
C6—C5—C8—O3	173.81 (17)	C6—C1—O5—C9	-14.8 (3)
C4—C5—C8—O4	174.98 (16)	C10—C9—O5—C1	-84.35 (19)

C6—C5—C8—O4 -6.4 (3)

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C10–C15 ring.

<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>
O2—H2 <i>A</i> ···O1 ⁱ	0.95 (3)	1.70 (3)	2.6426 (19)	176 (2)
O4—H4 <i>A</i> ···O7 ⁱⁱ	0.99 (3)	1.62 (3)	2.6086 (19)	175 (3)
O6—H6 <i>A</i> ···O3 ⁱⁱⁱ	0.93 (3)	1.72 (3)	2.6486 (19)	179 (4)
C9—H9 <i>A</i> ···O1 ^{iv}	0.97	2.51	3.272 (2)	135
C11—H11 <i>A</i> ···O3 ^v	0.93	2.45	3.170 (2)	135
C14—H14 <i>A</i> ···O4 ^{vi}	0.93	2.56	3.245 (2)	131
C9—H9 <i>B</i> ···Cg2 ^{vii}	0.97	2.97	3.779 (2)	141

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $x+1/2, y+1, -z+1/2$; (iii) $x-1/2, y-1, -z+1/2$; (iv) $-x+1, -y, -z$; (v) $-x+3/2, y-1/2, z$; (vi) $-x+1/2, y-1/2, z$; (vii) $-x+1/2, y+1/2, z$.