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Crystal structure and Hirshfeld surface analysis of 2-(4-nitrophenyl)-2-oxoethyl benzoate

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The title compound, $C_{15}H_{11}NO_5$, is relatively planar, with the planes of the two aromatic rings being inclined to each other by 3.09 (5)°. In the crystal, molecules are linked by a pair of C—H···O hydrogen bonds, forming inversion dimers, which enclose an $R_2^2(16)$ ring motif. The dimers are linked by a further pair of C—H···O hydrogen-bonds forming ribbons enclosing $R_4^4(26)$ ring motifs. The ribbons are linked by offset π–π interactions [centroid–centroid distances = 3.6754 (6)–3.7519 (6) Å] to form layers parallel to the *ac* plane. Through Hirshfeld surface analyses, the $d_{\rm norm}$ surfaces, electrostatic potential and two-dimensional fingerprint (FP) plots were examined to verify the contributions of the different intermolecular contacts within the supramolecular structure. The shape-index surface shows that two sides of the molecule are involved with the same contacts in neighbouring molecules, and the curvedness plot shows flat surface patches that are characteristic of planar stacking.

1. Chemical context

Photoreleasable protecting groups have been of long-standing interest for their diverse applications in various multistep syntheses (Ruzicka *et al.*, 2002; Literák *et al.*, 2006). The reaction between an acid and a phenacyl bromide yields the keto ester derivative. As a protecting group, the ester derivatives are well known as protecting groups for carboxylic acids in chemical synthesis (Rather & Reid, 1919; Literák *et al.*, 2006). They can easily be cleaved under completely neutral or mild conditions (Sheehan & Umezawa, 1973) and are therefore used for the identification of organic acids. Versatile applications of these compounds are seen in the field of synthetic chemistry, such as in the synthesis of oxazoles and imidazoles (Huang *et al.*, 1996), as well as benzoxazepine (Gandhi *et al.*, 1995), and they are also useful in peptide synthesis. Studies reveal an inhibitory activity against two isozymes of 11b-hydroxysteroid dehydrogenases (11b-HSD1 and 11b-HSD2), which catalyze the interconversion of active cortisol and inactive cortisone (Zhang *et al.*, 2009). Researchers have reported the synthesis and photolysis studies of a number of phenacyl esters. The commercial importance of phenacyl benzoates arose due to their applications in various fields of chemistry. In continuation of our work on such molecules (Kumar *et al.*, 2014; Chidan Kumar *et al.*, 2014), we report herein on the crystal and molecular structure of 2-(4-nitrophenyl)-2-oxoethyl benzoate.

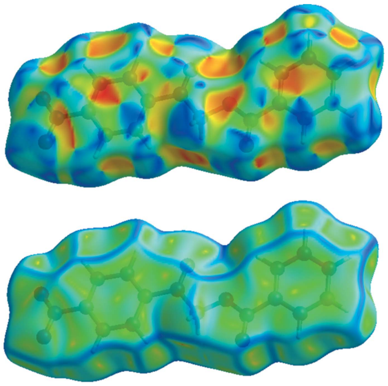

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Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3^{i}	0.95	2.47	3.3967 (14)	164
C13—H13···O5^{ii}	0.95	2.54	3.2361 (14)	130

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

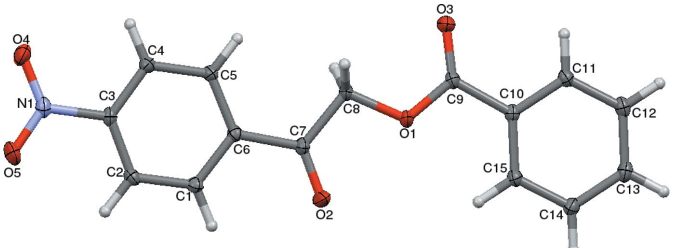
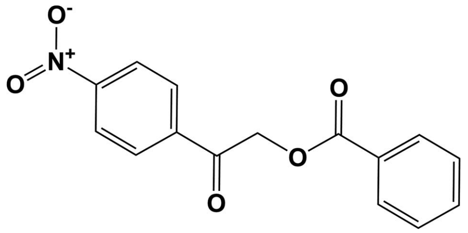


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.



2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The compound is composed of two aromatic rings linked by a C—C(=O)—O—C(=O) bridge. The unique molecular conformation of this compound is characterized by three torsion angles, *viz.* τ_1 (C11—C10—C9—O3), τ_2 (C7—C8—O1—C9) and τ_3 (O2—C7—C8—O1), whereby the τ_1 value of 9.60 (16)° signifies the apparent coplanarity between the mean planes of the phenyl ring and the adjacent carbonyl groups of the connecting bridge. The τ_2 value of 174.08 (9)° between the two carbonyl groups indicates an *antiperiplanar* conformation. Likewise, owing to a substitution on the functional group, the title compound experiences steric repulsion between the substituent and adjacent carbonyl groups, influencing the torsion angle [τ_3 = 1.88 (15)°], and it adopts a +*synperiplanar* conformation. The bond lengths and angles are normal and the molecular conformation is characterized by a dihedral angle of 3.09 (5)° between the mean planes of the two aromatic rings indicating that they are coplanar. The nitro group lies almost in the plane of the phenyl ring, as indicated by the torsion angle values of 7.80 (15) and 8.46 (15)° for C4—C3—N1—O4 and C2—C3—N1—O5, respectively.

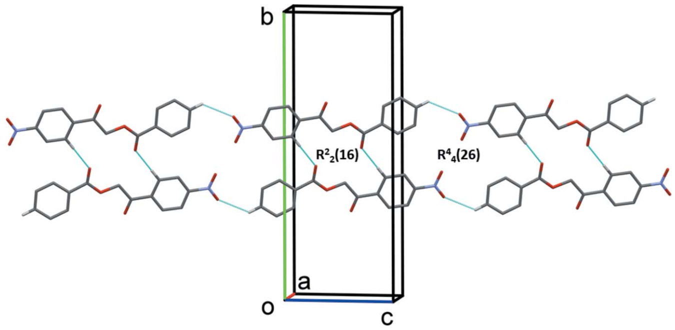


Figure 2
A partial view of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (Table 1) and only H atoms H5 and H13 have been included.

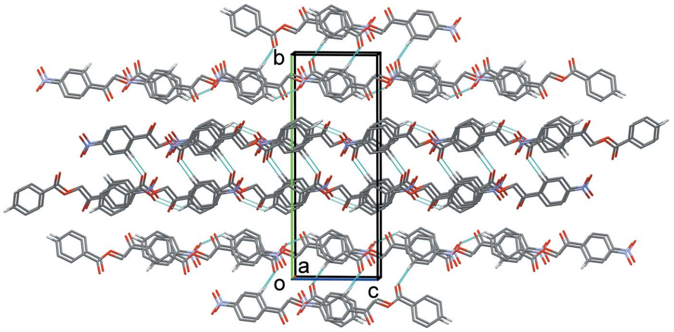


Figure 3
The crystal packing of the title compound, viewed along the *c* axis. The hydrogen bonds are shown as dashed lines (Table 1) and only H atoms H5 and H13 have been included.

3. Supramolecular features

In the crystal, there are no classical hydrogen bonds present. However, the structure is stabilized by weak intermolecular C—H···O interactions. Specifically, a pair of intermolecular C5—H5···O3^{i} interactions stabilize the supramolecular architecture by forming inversion dimers with an $R^2_2(16)$ ring motif (Table 1 and Fig. 2). The dimers are linked by a further pair of C—H···O hydrogen bonds, forming ribbons that enclose $R^4_4(26)$ ring motifs (Table 1 and Fig. 2). The ribbons are linked by a series of offset π–π interactions (Table 2), forming layers that stack up the *b*-axis direction (Fig. 3).

4. Hirshfeld surface analysis and two-dimensional fingerprint plots

The Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were performed and created with *CrystalExplorer17* (Turner *et al.*, 2017). Hirshfeld surface analysis enables the visualization of intermolecular interactions by different colours and colour intensity, representing short or long contacts and indicating the relative strengths of the interactions. Figs. 4 and 5 show the Hirshfeld surfaces mapped over d_{norm} (−0.195 to 1.091 a.u.) and shape-index (−1.0 to 1.0 a.u.), respectively.

In Fig. 4, the dark spots near the C and O atoms result from C—H···O interactions, which play a significant role in the molecular packing. The Hirshfeld surfaces illustrated in Fig. 4 also reflect the involvement of different atoms in the intermolecular interactions through the appearance of blue and red

Table 2
π–π contacts (Å, °) in the crystal of the title compound.

*Cg*1 and *Cg*2 are the centroids of rings C1–C6 and C10–C15, respectively.

$Cg(I)$	$Cg(J)$	$Cg(I)\cdots Cg(J)$ (Å)	α (°)	β (°)	γ (°)	*CgI*_Perp (Å)	*CgJ*_Perp (Å)	offset (Å)
*Cg*1	$Cg2^{\rm iii}$	3.6754 (6)	3.09 (5)	22.5	21.5	3.4199 (4)	3.3948 (4)	1.408
*Cg*1	$Cg2^{\rm iv}$	3.7519 (6)	3.09 (5)	27.9	25.1	3.3975 (4)	3.3171 (4)	1.753
*Cg*2	$Cg1^{\rm v}$	3.7519 (6)	3.09 (5)	25.1	27.9	3.3171 (4)	3.3975 (4)	1.592
*Cg*2	$Cg1^{\rm vi}$	3.6754 (6)	3.09 (5)	21.5	22.5	3.3948 (4)	3.4200 (4)	1.346

Symmetry codes: (iii) $x, y, z + 1$; (iv) $x + 1, y, z + 1$; (v) $x - 1, y, z - 1$; (vi) $x, y, z - 1$.

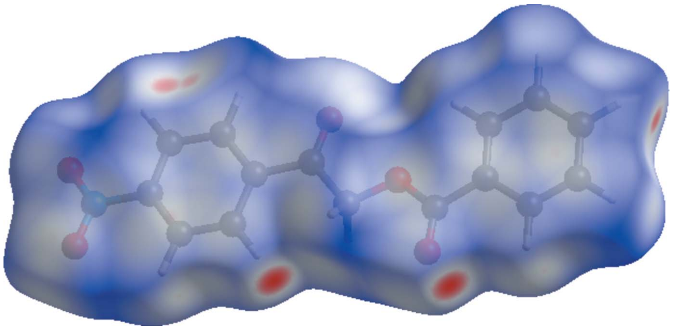


Figure 4
A view of the three-dimensional Hirshfeld surface of the title compound mapped over $d_{\rm norm}$.

regions around the participating atoms, which correspond to positive and negative electrostatic potential, respectively. The shape-index surface clearly shows that the two sides of the molecules are involved in the same contacts with neighbouring molecules and the curvedness plots show flat surface patches characteristic of planar stacking.

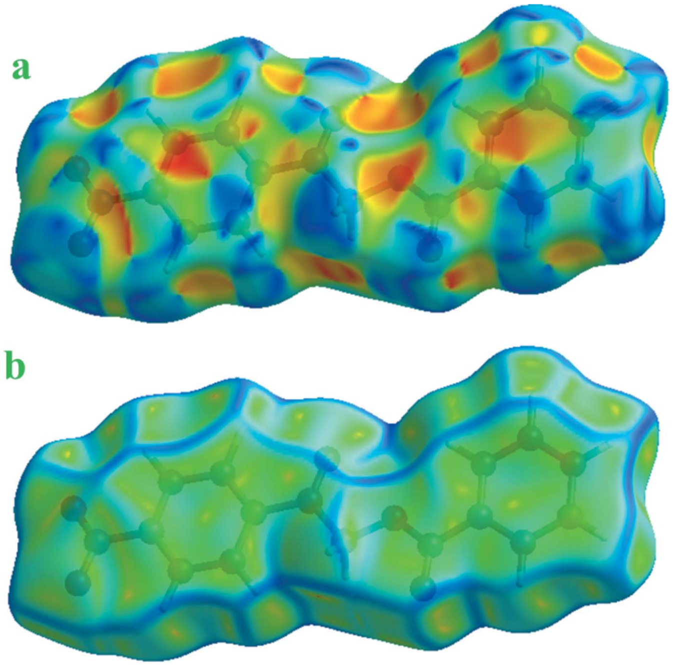


Figure 5
Hirshfeld surface of the title compound, mapped over (*a*) the shape-index and (*b*) the curvedness.

The overall two-dimensional fingerprint plot for the title compound and those delineated into O—H/H—O, H—H, C—H/H—C and C—C contacts are illustrated in Fig. 6. The percentage contributions from the different interatomic contacts to the Hirshfeld surfaces are O$\cdots$H = 35.9%, H$\cdots$H = 29.7%, C$\cdots$H = 14.7% and C$\cdots$C = 10.3%, and are shown in the two-dimensional fingerprint plots in Fig. 6. The percentage contributions of other intermolecular contacts are less than 5% in the Hirshfeld surface mapping.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, last update May 2019; Groom *et al.*, 2016) using 2-oxo-2-phenylethyl benzoate as the main skeleton revealed the presence of 62 structures with different substituents on the terminal phenyl rings (see supplementary information file S1).

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{11}NO_5$
M_r	285.25
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	7.3371 (4), 21.0051 (11), 8.3069 (4)
β (°)	102.711 (1)
V (Å^3)	1248.86 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.12
Crystal size (mm)	0.37 × 0.19 × 0.11
Data collection	
Diffractometer	Bruker APEXII DUO CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
$T_{\rm min}$, $T_{\rm max}$	0.959, 0.988
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14140, 3496, 3133
$R_{\rm int}$	0.029
$(\sin \theta/\lambda)_{\rm max}$ (Å^{-1})	0.708
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.120, 1.06
No. of reflections	3696
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.39, −0.30

Computer programs: *APEX2* (Bruker, 2012), *SAINT* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

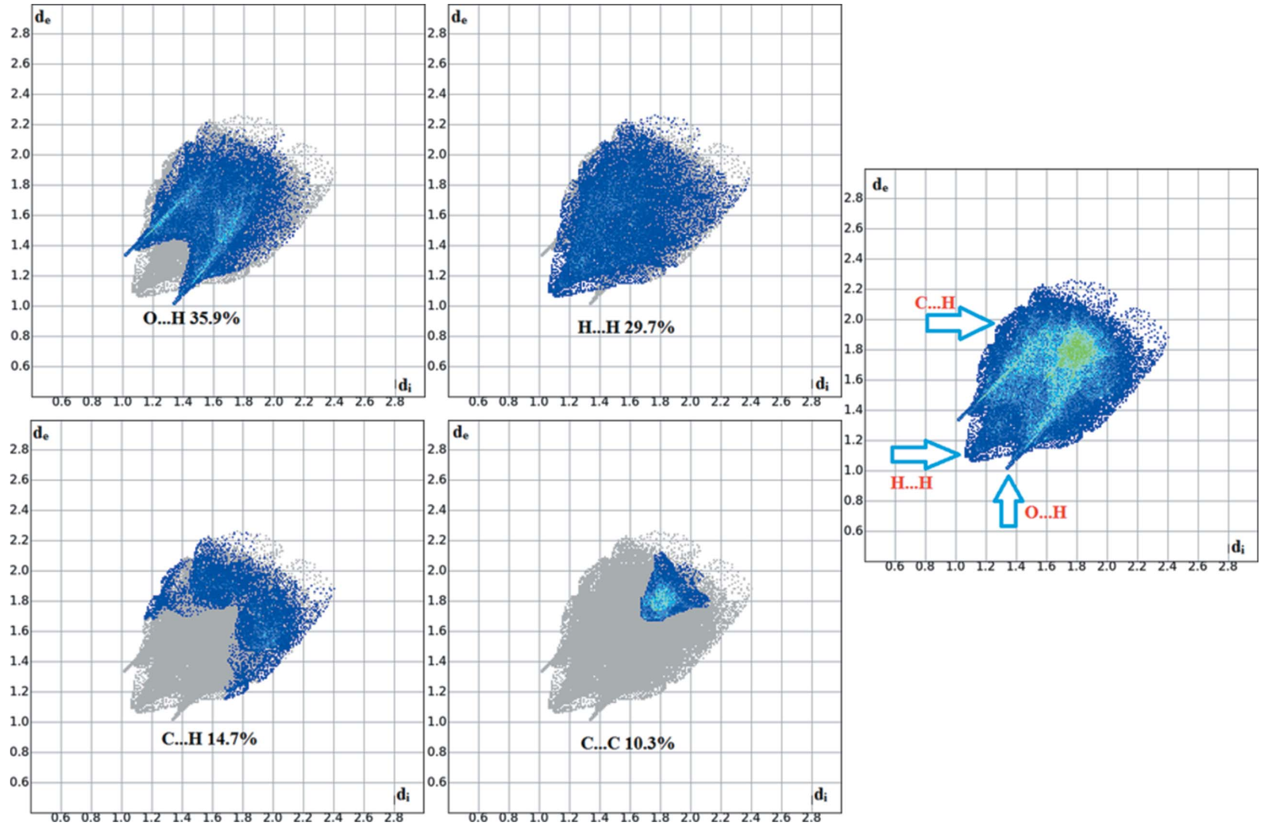


Figure 6
Two-dimensional fingerprint plots of the title compound, showing the percentage contributions of all contacts and of individual atom-atom contacts.

In these structures, the two aromatic rings are inclined to each other by dihedral angles varying from *ca* 0 to 90°. There are seven structures with a nitro substituent on one of the aromatic rings (see supplementary information file S2). However, there is only one compound with the same skeleton as the title compound, *i.e.* 2-(biphenyl-4-yl)-2-oxoethyl 4-nitrobenzoate (CSD refcode CISSAB; Kwong *et al.*, 2017). Here, the two aromatic rings are inclined to each other by *ca* 70.96°, compared to an inclination of only 3.09 (5)° in the title compound.

6. Synthesis and crystallization

The title compound was synthesized as per the procedure of Kumar *et al.* (2014). A mixture of 2-bromo-1-(4-nitrophenyl)ethanone (0.2 g, 0.5 mmol), potassium carbonate (0.087 g, 0.63 mmol) and benzoic acid (0.079 g, 0.65 mmol) in dimethylformamide (5 ml) was stirred at room temperature for 2 h. After completion of the reaction, the reaction mixture was poured into ice-cold water. The solid product obtained was filtered off, washed with water and recrystallized from ethanol to give colourless needle-like crystals (m.p. 386–390 K).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms on C atoms were positioned geometrically (C—H = 0.95–0.99 Å) and refined using a riding model, with $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$.

Acknowledgements

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supporting information

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Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

2-(4-Nitrophenyl)-2-oxoethyl benzoate

Crystal data

$C_{15}H_{11}NO_5$
$M_r = 285.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.3371$ (4) Å
$b = 21.0051$ (11) Å
$c = 8.3069$ (4) Å
$\beta = 102.711$ (1)°
$V = 1248.86$ (11) Å^3
$Z = 4$
$F(000) = 592$
$D_x = 1.517$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3133 reflections
$\theta = 1.9–30.2°$
$\mu = 0.12$ mm^{-1}
$T = 100$ K
Needle, colourless
0.37 × 0.19 × 0.11 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: Rotating Anode
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
$T_{\min} = 0.959$, $T_{\max} = 0.988$
14140 measured reflections
3496 independent reflections
3133 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.029$
$\theta_{\max} = 30.2°$, $\theta_{\min} = 1.9°$
$h = -10 \rightarrow 10$
$k = -29 \rightarrow 29$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.120$
$S = 1.06$
3696 reflections
190 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
$w = 1/[\sigma^2(F_o^2) + (0.0687P)^2 + 0.3119P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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}
O1	0.14827 (11)	0.38115 (4)	0.37625 (9)	0.0160 (2)
O2	0.34743 (16)	0.30646 (4)	0.58368 (11)	0.0357 (3)
O3	−0.02999 (13)	0.46698 (4)	0.29186 (10)	0.0227 (3)
O4	0.55675 (12)	0.44140 (4)	1.40112 (10)	0.0228 (2)
O5	0.70482 (14)	0.35199 (5)	1.40652 (11)	0.0292 (3)
N1	0.59732 (13)	0.39281 (5)	1.33492 (11)	0.0167 (2)
C1	0.47223 (14)	0.31711 (5)	0.92088 (13)	0.0142 (3)
C2	0.54458 (14)	0.32506 (5)	1.08833 (13)	0.0142 (3)
C3	0.51595 (14)	0.38305 (5)	1.15843 (12)	0.0129 (2)
C4	0.41568 (14)	0.43237 (5)	1.06970 (13)	0.0137 (2)
C5	0.34479 (14)	0.42390 (5)	0.90160 (12)	0.0128 (2)
C6	0.37472 (13)	0.36653 (5)	0.82655 (12)	0.0123 (2)
C7	0.30848 (15)	0.35532 (5)	0.64525 (13)	0.0152 (3)
C8	0.19380 (15)	0.40611 (5)	0.54070 (12)	0.0144 (3)
C9	0.03139 (14)	0.41587 (5)	0.26299 (12)	0.0132 (2)
C10	−0.01390 (13)	0.38341 (5)	0.09985 (12)	0.0122 (2)
C11	−0.11222 (14)	0.41756 (5)	−0.03566 (13)	0.0140 (3)
C12	−0.16055 (14)	0.38880 (5)	−0.18959 (13)	0.0159 (3)
C13	−0.11199 (15)	0.32571 (5)	−0.20797 (13)	0.0168 (3)
C14	−0.01248 (15)	0.29164 (5)	−0.07323 (13)	0.0162 (3)
C15	0.03811 (14)	0.32043 (5)	0.08058 (13)	0.0138 (3)
H1	0.48900	0.27770	0.86970	0.0170*
H2	0.61170	0.29180	1.15300	0.0170*
H4	0.39580	0.47110	1.12250	0.0160*
H5	0.27610	0.45710	0.83790	0.0150*
H8A	0.07880	0.41510	0.58050	0.0170*
H8B	0.26650	0.44600	0.54450	0.0170*
H11	−0.14620	0.46060	−0.02260	0.0170*
H12	−0.22660	0.41220	−0.28210	0.0190*
H13	−0.14680	0.30570	−0.31290	0.0200*
H14	0.02090	0.24860	−0.08660	0.0190*
H15	0.10770	0.29740	0.17220	0.0170*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0200 (4)	0.0170 (4)	0.0090 (3)	0.0052 (3)	−0.0008 (3)	−0.0008 (3)
O2	0.0581 (7)	0.0226 (4)	0.0179 (4)	0.0205 (4)	−0.0097 (4)	−0.0078 (3)
O3	0.0325 (5)	0.0174 (4)	0.0160 (4)	0.0090 (3)	0.0003 (3)	−0.0014 (3)
O4	0.0256 (4)	0.0266 (4)	0.0150 (4)	0.0018 (3)	0.0018 (3)	−0.0064 (3)
O5	0.0366 (5)	0.0313 (5)	0.0149 (4)	0.0113 (4)	−0.0048 (4)	0.0036 (3)
N1	0.0159 (4)	0.0219 (4)	0.0115 (4)	0.0000 (3)	0.0015 (3)	0.0007 (3)
C1	0.0155 (5)	0.0123 (4)	0.0142 (5)	−0.0001 (3)	0.0017 (4)	0.0004 (3)
C2	0.0142 (5)	0.0138 (4)	0.0137 (5)	0.0008 (3)	0.0012 (4)	0.0032 (3)
C3	0.0120 (4)	0.0171 (4)	0.0093 (4)	−0.0018 (3)	0.0015 (3)	0.0007 (3)
C4	0.0142 (4)	0.0138 (4)	0.0128 (4)	0.0007 (3)	0.0026 (4)	−0.0012 (3)
C5	0.0130 (4)	0.0128 (4)	0.0119 (4)	0.0016 (3)	0.0010 (3)	0.0007 (3)
C6	0.0117 (4)	0.0126 (4)	0.0119 (4)	−0.0012 (3)	0.0012 (3)	−0.0005 (3)
C7	0.0171 (5)	0.0145 (4)	0.0120 (4)	0.0007 (4)	−0.0012 (4)	−0.0007 (3)
C8	0.0184 (5)	0.0149 (4)	0.0089 (4)	0.0024 (4)	0.0010 (4)	−0.0004 (3)
C9	0.0139 (4)	0.0142 (4)	0.0112 (4)	−0.0001 (3)	0.0020 (4)	0.0019 (3)
C10	0.0115 (4)	0.0144 (4)	0.0106 (4)	−0.0010 (3)	0.0021 (3)	0.0002 (3)
C11	0.0136 (4)	0.0151 (4)	0.0129 (5)	0.0012 (3)	0.0022 (4)	0.0021 (3)
C12	0.0142 (5)	0.0207 (5)	0.0118 (5)	−0.0004 (4)	0.0007 (4)	0.0030 (4)
C13	0.0180 (5)	0.0209 (5)	0.0109 (4)	−0.0024 (4)	0.0022 (4)	−0.0011 (4)
C14	0.0203 (5)	0.0156 (5)	0.0128 (5)	0.0002 (4)	0.0041 (4)	−0.0012 (4)
C15	0.0157 (5)	0.0142 (4)	0.0113 (4)	0.0004 (3)	0.0027 (4)	0.0015 (3)

Geometric parameters (Å, º)

O1—C8	1.4324 (12)	C10—C15	1.3958 (15)
O1—C9	1.3407 (13)	C11—C12	1.3879 (15)
O2—C7	1.2087 (14)	C12—C13	1.3894 (15)
O3—C9	1.2085 (14)	C13—C14	1.3923 (15)
O4—N1	1.2267 (13)	C14—C15	1.3883 (15)
O5—N1	1.2266 (14)	C1—H1	0.9500
N1—C3	1.4706 (13)	C2—H2	0.9500
C1—C2	1.3855 (15)	C4—H4	0.9500
C1—C6	1.3988 (15)	C5—H5	0.9500
C2—C3	1.3859 (15)	C8—H8A	0.9900
C3—C4	1.3853 (15)	C8—H8B	0.9900
C4—C5	1.3901 (14)	C11—H11	0.9500
C5—C6	1.3962 (15)	C12—H12	0.9500
C6—C7	1.4959 (14)	C13—H13	0.9500
C7—C8	1.5096 (15)	C14—H14	0.9500
C9—C10	1.4878 (14)	C15—H15	0.9500
C10—C11	1.3945 (14)		
C8—O1—C9	116.69 (8)	C12—C13—C14	120.25 (10)
O4—N1—O5	123.90 (9)	C13—C14—C15	120.18 (10)
O4—N1—C3	118.53 (9)	C10—C15—C14	119.60 (10)

O5—N1—C3	117.56 (9)	C2—C1—H1	120.00
C2—C1—C6	120.58 (10)	C6—C1—H1	120.00
C1—C2—C3	117.89 (10)	C1—C2—H2	121.00
N1—C3—C2	118.40 (9)	C3—C2—H2	121.00
N1—C3—C4	118.54 (9)	C3—C4—H4	121.00
C2—C3—C4	123.06 (9)	C5—C4—H4	121.00
C3—C4—C5	118.44 (10)	C4—C5—H5	120.00
C4—C5—C6	119.88 (9)	C6—C5—H5	120.00
C1—C6—C5	120.11 (9)	O1—C8—H8A	111.00
C1—C6—C7	117.39 (9)	O1—C8—H8B	111.00
C5—C6—C7	122.50 (9)	C7—C8—H8A	111.00
O2—C7—C6	120.33 (10)	C7—C8—H8B	111.00
O2—C7—C8	120.69 (10)	H8A—C8—H8B	109.00
C6—C7—C8	118.98 (9)	C10—C11—H11	120.00
O1—C8—C7	105.87 (8)	C12—C11—H11	120.00
O1—C9—O3	123.56 (9)	C11—C12—H12	120.00
O1—C9—C10	111.72 (9)	C13—C12—H12	120.00
O3—C9—C10	124.72 (9)	C12—C13—H13	120.00
C9—C10—C11	118.15 (9)	C14—C13—H13	120.00
C9—C10—C15	121.80 (9)	C13—C14—H14	120.00
C11—C10—C15	120.06 (9)	C15—C14—H14	120.00
C10—C11—C12	120.11 (10)	C10—C15—H15	120.00
C11—C12—C13	119.78 (10)	C14—C15—H15	120.00

C9—O1—C8—C7	174.08 (9)	C1—C6—C7—C8	176.74 (10)
C8—O1—C9—O3	2.69 (15)	C5—C6—C7—O2	175.36 (11)
C8—O1—C9—C10	−176.70 (9)	C5—C6—C7—C8	−4.18 (15)
O4—N1—C3—C2	−172.74 (10)	O2—C7—C8—O1	1.88 (15)
O4—N1—C3—C4	7.80 (15)	C6—C7—C8—O1	−178.58 (9)
O5—N1—C3—C2	8.46 (15)	O1—C9—C10—C11	−171.02 (9)
O5—N1—C3—C4	−171.00 (10)	O1—C9—C10—C15	9.44 (14)
C6—C1—C2—C3	0.43 (16)	O3—C9—C10—C11	9.60 (16)
C2—C1—C6—C5	−1.83 (16)	O3—C9—C10—C15	−169.95 (11)
C2—C1—C6—C7	177.27 (10)	C9—C10—C11—C12	−178.79 (10)
C1—C2—C3—N1	−178.03 (9)	C15—C10—C11—C12	0.77 (15)
C1—C2—C3—C4	1.41 (16)	C9—C10—C15—C14	178.01 (10)
N1—C3—C4—C5	177.65 (9)	C11—C10—C15—C14	−1.52 (15)
C2—C3—C4—C5	−1.79 (16)	C10—C11—C12—C13	0.53 (16)
C3—C4—C5—C6	0.33 (15)	C11—C12—C13—C14	−1.06 (16)
C4—C5—C6—C1	1.43 (15)	C12—C13—C14—C15	0.30 (17)
C4—C5—C6—C7	−177.62 (10)	C13—C14—C15—C10	0.99 (16)
C1—C6—C7—O2	−3.72 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O3$^{\mathrm{i}}$	0.95	2.47	3.3967 (14)	164

C13—H13···O5$^{\text{ii}}$	0.95	2.54	3.2361 (14)	130

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