research communications

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

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The title compound, $C_{15}H_{10}ClNO_5$, is relatively planar with the two aromatic rings being inclined to each other by 3.56 (11)°. The central —C(═O)—C–O—C(═O)— bridge is slightly twisted, with a C—C—O—C torsion angle of 164.95 (16)°. In the crystal, molecules are linked by C—H⋯O and C—H⋯Cl hydrogen bonds, forming layers parallel to the (101) plane. The layers are linked by a further C—H⋯O hydrogen bond, forming a three-dimensional supramolecular structure. There are a number of offset π–π interactions present between the layers [intercentroid distances vary from 3.8264 (15) to 3.9775 (14) Å]. Hirshfeld surface analyses, the d_{norm} surfaces, electrostatic potential and two-dimensional fingerprint 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 in the same contacts with neighbouring molecules, and the curvedness plot shows flat surface patches that are characteristic of planar stacking.

1. Chemical context

Due to their numerous applications in various fields of chemistry, phenacyl benzoates are of great importance (Rather & Reid, 1919; Literák *et al.*, 2006; Sheehan & Umezawa, 1973; Huang *et al.*, 1996; Gandhi *et al.*, 1995; Zhang *et al.*, 2009). 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 structures of 2-(4-nitrophenyl)-2-oxoethyl chlorobenzoate (I). Its crystal and molecular structures are compared with those of 2-(4-nitrophenyl)-2-oxoethyl benzoate (II) (Sheshadri *et al.*, 2019), published by us recently, and further details of uses and applications of such molecules are described therein.

2. Structural commentary

The molecular structure of the title compound, I, is shown in Fig. 1. The compound is composed of two aromatic rings (C1–C6 and C10–C15) linked by the –C7(═O2)—C8—O1—C9(═O3)– bridge. The bond lengths and angles in I are normal and similar to those reported for compound II. The two benzene rings are inclined to each other by 3.56 (11)°, indicating that they are almost coplanar, as in the structure of II. The nitro group (N1/O4/O5) lies almost in the plane of the benzene ring (C1–C6), with a dihedral angle between the two
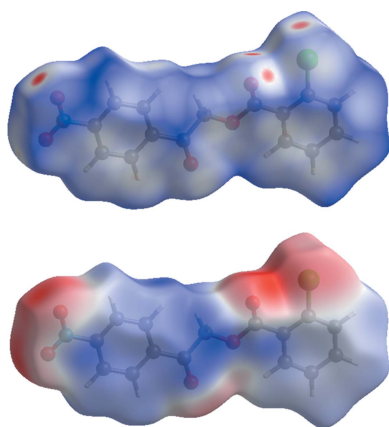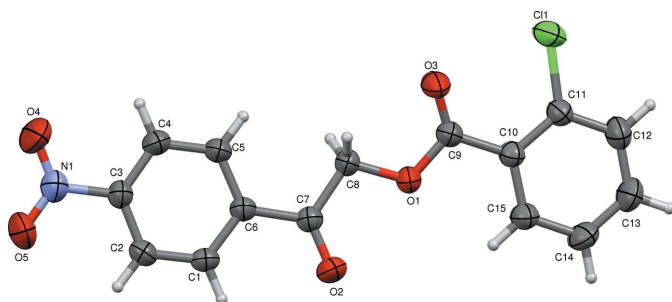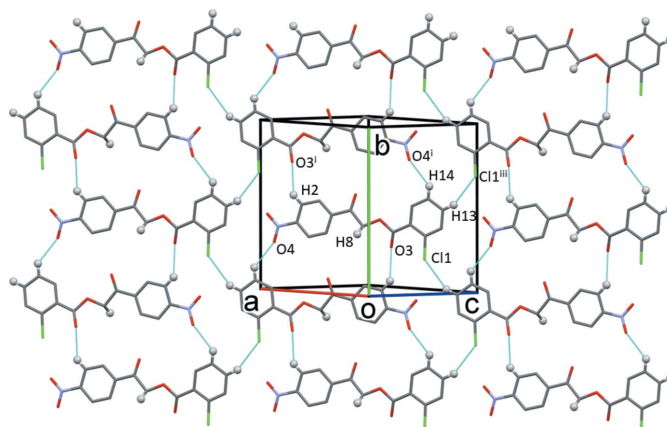
Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2$\cdots$O3^i	0.93	2.54	3.258 (2)	135
C8—H8$A\cdots$O3^{ii}	0.97	2.59	3.553 (3)	171
C13—H13$\cdots$Cl1^{iii}	0.93	2.82	3.670 (3)	153
C14—H14$\cdots$O4^i	0.93	2.50	3.211 (4)	134

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

planes of 5.4 (4)°; the torsion angles C4—C3—N1—O4 and C2—C3—N1—O5 are −5.4 (3) and −5.1 (4)°, respectively. Atom Cl1 is displaced by 0.0749 (8) Å from the plane of benzene ring C10–C15.

(I) X = Cl
(II) X = H
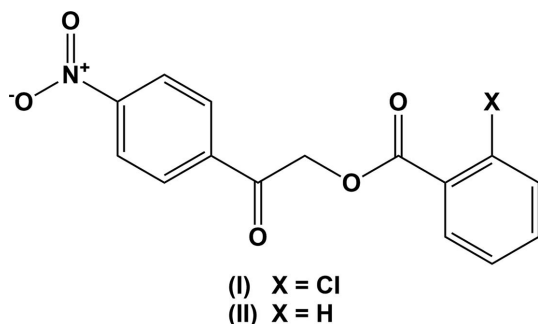
The overall molecular conformation of I is characterized by three torsion angles, viz. τ_1 (C11—C10—C9—O3), τ_2 (C7—C8—O1—C9) and τ_3 (O2—C7—C6—C1). Torsion angle τ_1 at −12.5 (3)° signifies a certain noncoplanarity between the benzene ring (C10–C15) and the adjacent carbonyl group (C9=O3) as a result of steric repulsion between the substituent Cl1 and the adjacent carbonyl group C9=O3. This is also reflected in the torsion angle τ_2 of −164.95 (16)°, between the two carbonyl groups, C7=O2 and C9=O3, which have a –antiperiplanar conformation. Torsion angle τ_3, involving the benzene ring (C1–C6) and the adjacent carbonyl group (C7=O2), is −3.6 (3)° and indicates a –synperiplanar conformation. A comparison of the torsion angles in I and II, indicates that the insertion of the Cl atom in I has the most significant influence on torsion τ_2, which is −164.95 (16)° in I compared to 174.08 (9)° in II. Torsion angles τ_1 of −12.5 (3)° and τ_3 of −3.6 (3)° are slightly larger than the values observed in II, viz. 9.60 (16) and 1.88 (15)°, respectively. Hence,

Figure 2
A view normal to the (101) plane of the crystal packing of compound I. The hydrogen bonds are shown as dashed lines (Table 1; symmetry codes as in Table 1), and, for clarity, only the H atoms involved in hydrogen bonding have been included.

compound I has a less planar conformation than unsubstituted compound II.

3. Supramolecular features

The crystal structure of the title compound, is stabilized by intermolecular hydrogen bonds of the types C—H$\cdots$O and C—H$\cdots$Cl (Table 1). Molecules are linked by the C2—H2$\cdots$O3^i, C14—H14$\cdots$O4^i and C13—H13$\cdots$Cl1^{iii} hydrogen bonds to form layers lying parallel to the (101) plane; see Fig. 2 and Table 1. The layers are linked by C8—H8$A\cdots$O3^{ii} hydrogen bonds and offset π–π interactions (see Table 2), forming a supramolecular three-dimensional structure (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 with Crystal-

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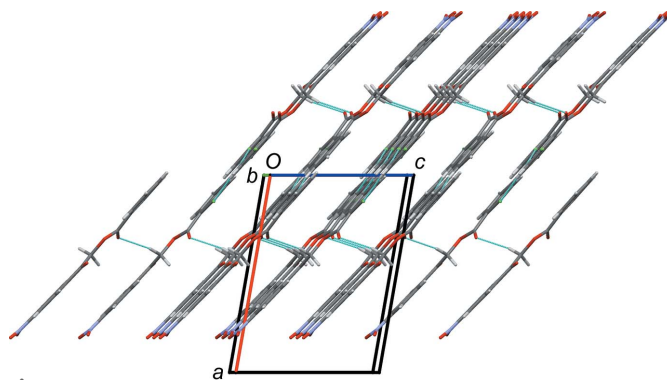

Figure 3
The crystal packing of compound I, viewed along the b axis, showing the layered stacking. For clarity, only the H atoms involved in hydrogen bonding have been included, and the hydrogen bonds are shown as dashed lines (Table 1).

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

Cg1 and Cg2 are the centroids of the C1–C6 and C10–C15 rings, respectively.

$Cg(I)$	$Cg(J)$	$Cg(I)\cdots Cg(J)$ (Å)	α (°)	β (°)	γ (°)	CgI_Perp (Å)	CgJ_Perp (Å)	Offset (Å)
Cg1	Cg1[iv]	3.9775 (14)	0.02 (10)	31.8	31.8	3.3791 (9)	3.3791 (9)	2.098
Cg1	Cg2[v]	3.8801 (14)	3.56 (11)	30.1	29.1	3.3895 (9)	3.3559 (10)	1.948
Cg2	Cg2[vi]	3.8264 (15)	0.00 (11)	24.8	24.8	3.4722 (10)	3.4722 (10)	1.608

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

Explorer17 (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 strength of the interactions. Fig. 4(*a*) shows the Hirshfeld surface mapped over d_{norm} (−0.154 to 1.305) and for Fig. 4(*b*) the electrostatic potential. The Hirshfeld surface illustrated in Fig. 4(*a*) reflects the involvement of different atoms with the intermolecular interactions through the appearance of blue and red patches, which correspond to the regions of positive and negative electrostatic potential shown in Fig. 4(*b*). The shape-index surface (Fig. 5*a*) clearly shows that the two sides of the molecule are involved in contacts with neighbouring molecules and the curvedness plot (Fig. 5*b*) shows flat surface patches characteristic of planar stacking.

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 Cl···H/H···Cl contacts are illustrated in Fig. 6. The percentage contributions from the different interatomic contacts to the Hirshfeld surfaces are as follows: O···H (34.8%), H···H (18.8%), C···H (14.7%) and Cl···H (10.1%),

shown in the two-dimensional fingerprint plots, respectively, in Fig. 6. The percentage contributions for 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. In these structures, the two aromatic rings are inclined to each other by dihedral angles varying from *ca* 0 to 90°. There were seven structures with a nitro substituent on one of the aromatic rings. 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 only 3.56 (11)° in the title compound. In the crystal structure of the recently published compound 2-(4-

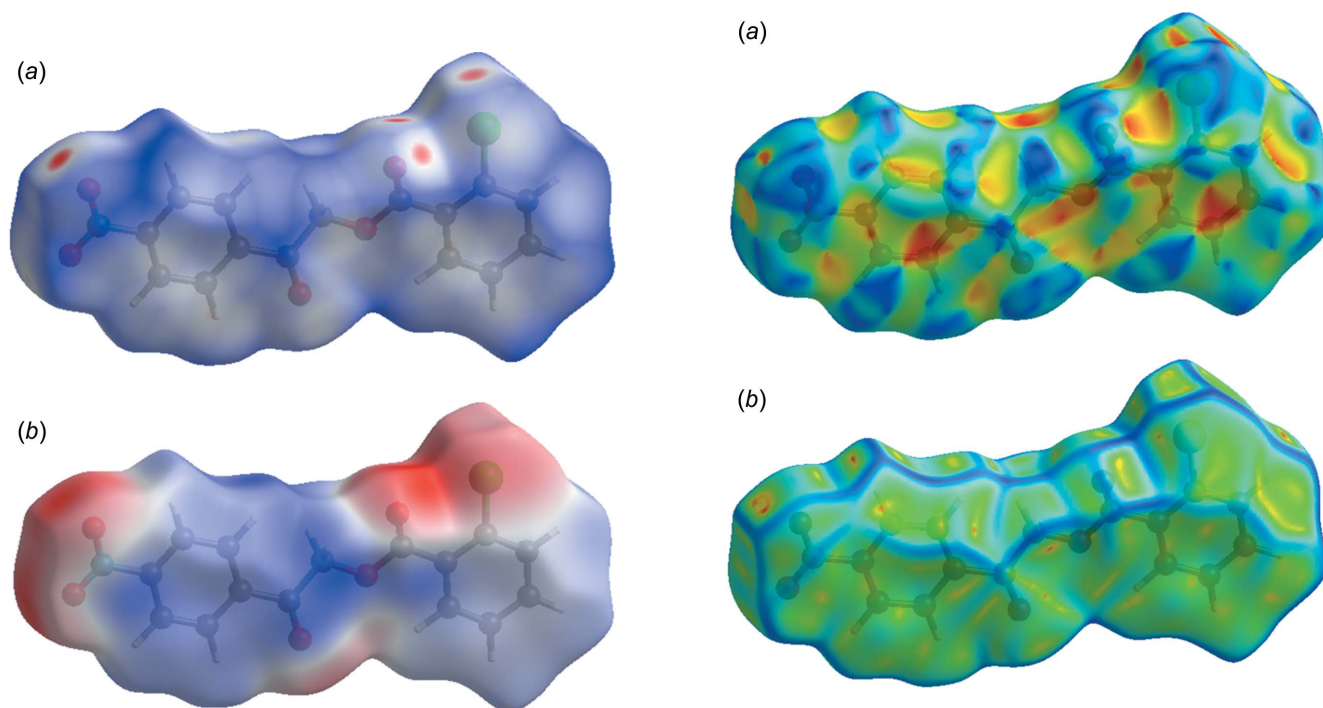**Figure 4**
A view of the Hirshfeld surface of compound I, mapped over d_{norm}.

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

nitrophenyl)-2-oxoethyl benzoate (II) (Sheshadri *et al.*, 2019), this dihedral angle is 3.09 (5)°.

6. Synthesis and crystallization

The title compound, was synthesized as per the procedure reported earlier by 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 2-chlorobenzoic acid (0.156 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, washed with water and recrystallized from ethanol to give colourless block-like crystals (m.p. 386–390 K).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Acknowledgements

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Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}ClNO_5$
M_r	319.69
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	294
a, b, c (Å)	12.6646 (18), 12.4099 (18), 9.0902 (13)
β (°)	99.947 (2)
V (Å^3)	1407.2 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.30
Crystal size (mm)	$0.55 \times 0.26 \times 0.19$
Data collection	
Diffractometer	Bruker APEXII DUO CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.796, 0.946
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36449, 4122, 2586
R_{int}	0.058
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.705
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.141, 1.06
No. of reflections	4122
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.26, −0.44

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).
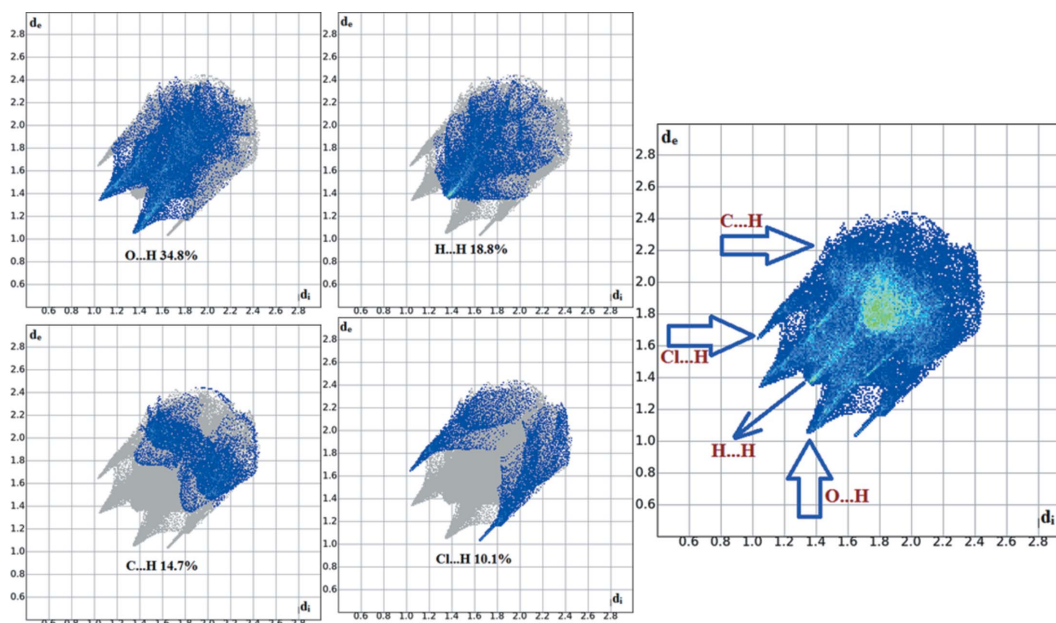

Figure 6
The two-dimensional fingerprint plots of compound I, showing the percentage contributions of all contacts and of individual atom–atom contacts.

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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 2-chlorobenzoate

Crystal data

$C_{15}H_{10}ClNO_5$	$F(000) = 656$
$M_r = 319.69$	$D_x = 1.509$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 6264 reflections
$a = 12.6646$ (18) Å	$\theta = 2.3$–27.5°
$b = 12.4099$ (18) Å	$\mu = 0.30$ mm^{-1}
$c = 9.0902$ (13) Å	$T = 294$ K
$\beta = 99.947$ (2)°	Block, colourless
$V = 1407.2$ (3) Å^3	$0.55 \times 0.26 \times 0.19$ mm
$Z = 4$	

Data collection

Bruker APEXII DUO CCD area-detector diffractometer	36449 measured reflections
Radiation source: Rotating Anode	4122 independent reflections
Graphite monochromator	2586 reflections with $I > 2\sigma(I)$
Detector resolution: 18.4 pixels mm^{-1}	$R_{int} = 0.058$
φ and ω scans	$\theta_{max} = 30.1°$, $\theta_{min} = 1.6°$
Absorption correction: multi-scan (SADABS; Bruker, 2012)	$h = -17 \rightarrow 17$
	$k = -17 \rightarrow 17$
$T_{min} = 0.796$, $T_{max} = 0.946$	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	199 parameters
Least-squares matrix: full	0 restraints
$R[F^2 > 2\sigma(F^2)] = 0.054$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.141$	
$S = 1.06$	H-atom parameters constrained
4122 reflections	

$W = 1/[\Sigma^2(FO^2) + (0.0456P)^2 + 0.8032P]$
    WHERE $P = (FO^2 + 2FC^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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 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 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 (Å²)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Cl1	0.13276 (6)	0.19871 (4)	0.64688 (9)	0.0704 (3)
O1	0.32241 (12)	0.43016 (11)	0.42430 (17)	0.0451 (5)
O2	0.44530 (13)	0.57459 (11)	0.32308 (19)	0.0553 (6)
O3	0.31616 (15)	0.26717 (12)	0.5238 (2)	0.0662 (7)
O4	0.8091 (3)	0.28826 (18)	−0.0648 (4)	0.1349 (15)
O5	0.8233 (2)	0.45298 (17)	−0.1127 (3)	0.1031 (10)
N1	0.78442 (18)	0.38048 (17)	−0.0532 (3)	0.0632 (8)
C1	0.60280 (16)	0.53537 (15)	0.1467 (2)	0.0378 (6)
C2	0.68013 (17)	0.51241 (15)	0.0615 (2)	0.0407 (6)
C3	0.70239 (17)	0.40590 (16)	0.0379 (2)	0.0432 (7)
C4	0.65143 (19)	0.32166 (16)	0.0961 (3)	0.0493 (7)
C5	0.57408 (18)	0.34589 (15)	0.1802 (3)	0.0458 (7)
C6	0.54870 (15)	0.45265 (14)	0.2066 (2)	0.0356 (6)
C7	0.46407 (16)	0.48220 (15)	0.2957 (2)	0.0367 (6)
C8	0.40417 (18)	0.38936 (16)	0.3492 (2)	0.0429 (6)
C9	0.28099 (17)	0.35666 (15)	0.5069 (2)	0.0394 (6)
C10	0.19286 (15)	0.40267 (15)	0.5758 (2)	0.0365 (6)
C11	0.12673 (17)	0.33809 (16)	0.6478 (2)	0.0414 (6)
C12	0.05046 (19)	0.3840 (2)	0.7205 (3)	0.0548 (8)
C13	0.0388 (2)	0.4942 (2)	0.7222 (3)	0.0604 (9)
C14	0.10067 (19)	0.55891 (18)	0.6499 (3)	0.0544 (8)
C15	0.17715 (17)	0.51397 (16)	0.5769 (3)	0.0443 (7)
H1	0.58650	0.60680	0.16450	0.0450*
H2	0.71620	0.56730	0.02110	0.0490*
H4	0.66890	0.25050	0.07900	0.0590*
H5	0.53830	0.29040	0.21980	0.0550*
H8A	0.37220	0.34550	0.26490	0.0510*
H8B	0.45330	0.34460	0.41680	0.0510*
H12	0.00710	0.34040	0.76810	0.0660*
H13	−0.01150	0.52480	0.77300	0.0720*
H14	0.09130	0.63320	0.64990	0.0650*
H15	0.21870	0.55860	0.52770	0.0530*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0741 (4)	0.0363 (3)	0.1119 (6)	−0.0032 (3)	0.0471 (4)	0.0109 (3)
O1	0.0529 (9)	0.0353 (7)	0.0540 (9)	0.0031 (6)	0.0285 (7)	0.0035 (6)
O2	0.0648 (11)	0.0323 (7)	0.0754 (11)	−0.0003 (7)	0.0311 (9)	−0.0077 (7)
O3	0.0755 (12)	0.0382 (8)	0.0983 (14)	0.0158 (8)	0.0524 (11)	0.0190 (8)
O4	0.165 (3)	0.0587 (13)	0.222 (3)	0.0172 (14)	0.149 (3)	−0.0060 (16)
O5	0.1241 (19)	0.0699 (13)	0.144 (2)	−0.0058 (13)	0.1036 (18)	0.0043 (13)
N1	0.0670 (14)	0.0509 (11)	0.0825 (16)	−0.0031 (10)	0.0433 (12)	−0.0073 (11)
C1	0.0436 (11)	0.0268 (8)	0.0437 (11)	−0.0021 (7)	0.0095 (9)	−0.0019 (8)
C2	0.0446 (11)	0.0342 (9)	0.0456 (12)	−0.0058 (8)	0.0141 (9)	0.0031 (8)
C3	0.0444 (12)	0.0394 (10)	0.0504 (13)	−0.0019 (9)	0.0214 (10)	−0.0037 (9)
C4	0.0588 (14)	0.0296 (9)	0.0659 (15)	−0.0004 (9)	0.0284 (12)	−0.0048 (9)
C5	0.0554 (13)	0.0288 (9)	0.0591 (14)	−0.0051 (9)	0.0268 (11)	−0.0009 (9)
C6	0.0393 (10)	0.0295 (8)	0.0392 (11)	−0.0031 (7)	0.0106 (9)	−0.0026 (8)
C7	0.0412 (11)	0.0320 (9)	0.0383 (11)	−0.0015 (8)	0.0105 (9)	−0.0013 (8)
C8	0.0517 (12)	0.0341 (9)	0.0486 (12)	0.0005 (8)	0.0250 (10)	−0.0021 (8)
C9	0.0428 (11)	0.0322 (9)	0.0458 (12)	−0.0011 (8)	0.0149 (9)	0.0010 (8)
C10	0.0355 (10)	0.0339 (9)	0.0410 (11)	0.0012 (7)	0.0089 (9)	0.0032 (8)
C11	0.0409 (11)	0.0368 (9)	0.0491 (12)	−0.0001 (8)	0.0149 (9)	0.0046 (9)
C12	0.0500 (13)	0.0566 (13)	0.0644 (16)	0.0006 (11)	0.0288 (12)	0.0066 (12)
C13	0.0540 (14)	0.0560 (14)	0.0790 (18)	0.0104 (11)	0.0336 (14)	−0.0026 (13)
C14	0.0537 (14)	0.0369 (11)	0.0762 (17)	0.0096 (9)	0.0214 (13)	−0.0022 (10)
C15	0.0456 (12)	0.0343 (10)	0.0553 (13)	0.0018 (8)	0.0150 (10)	0.0030 (9)

Geometric parameters (Å, °)

Cl1—C11	1.732 (2)	C10—C11	1.401 (3)
O1—C8	1.428 (3)	C10—C15	1.396 (3)
O1—C9	1.344 (2)	C11—C12	1.384 (3)
O2—C7	1.206 (2)	C12—C13	1.376 (4)
O3—C9	1.197 (2)	C13—C14	1.367 (4)
O4—N1	1.196 (3)	C14—C15	1.383 (3)
O5—N1	1.199 (3)	C1—H1	0.9300
N1—C3	1.470 (3)	C2—H2	0.9300
C1—C2	1.379 (3)	C4—H4	0.9300
C1—C6	1.396 (3)	C5—H5	0.9300
C2—C3	1.376 (3)	C8—H8A	0.9700
C3—C4	1.381 (3)	C8—H8B	0.9700
C4—C5	1.376 (3)	C12—H12	0.9300
C5—C6	1.394 (3)	C13—H13	0.9300
C6—C7	1.496 (3)	C14—H14	0.9300
C7—C8	1.506 (3)	C15—H15	0.9300
C9—C10	1.485 (3)		
C8—O1—C9	114.31 (15)	C10—C11—C12	120.71 (19)
O4—N1—O5	123.0 (3)	C11—C12—C13	120.0 (2)

O4—N1—C3	118.4 (3)	C12—C13—C14	120.5 (2)
O5—N1—C3	118.6 (2)	C13—C14—C15	120.1 (2)
C2—C1—C6	120.74 (17)	C10—C15—C14	121.0 (2)
C1—C2—C3	118.07 (18)	C2—C1—H1	120.00
N1—C3—C2	118.53 (18)	C6—C1—H1	120.00
N1—C3—C4	118.41 (19)	C1—C2—H2	121.00
C2—C3—C4	123.1 (2)	C3—C2—H2	121.00
C3—C4—C5	118.17 (19)	C3—C4—H4	121.00
C4—C5—C6	120.72 (19)	C5—C4—H4	121.00
C1—C6—C5	119.24 (18)	C4—C5—H5	120.00
C1—C6—C7	118.47 (16)	C6—C5—H5	120.00
C5—C6—C7	122.29 (18)	O1—C8—H8A	110.00
O2—C7—C6	122.01 (18)	O1—C8—H8B	110.00
O2—C7—C8	122.19 (19)	C7—C8—H8A	110.00
C6—C7—C8	115.80 (16)	C7—C8—H8B	110.00
O1—C8—C7	109.30 (16)	H8A—C8—H8B	108.00
O1—C9—O3	121.9 (2)	C11—C12—H12	120.00
O1—C9—C10	111.65 (16)	C13—C12—H12	120.00
O3—C9—C10	126.36 (19)	C12—C13—H13	120.00
C9—C10—C11	122.06 (17)	C14—C13—H13	120.00
C9—C10—C15	120.13 (18)	C13—C14—H14	120.00
C11—C10—C15	117.74 (18)	C15—C14—H14	120.00
Cl1—C11—C10	122.61 (16)	C10—C15—H15	120.00
Cl1—C11—C12	116.66 (17)	C14—C15—H15	119.00
C9—O1—C8—C7	−164.95 (16)	C5—C6—C7—O2	177.1 (2)
C8—O1—C9—O3	5.3 (3)	C5—C6—C7—C8	−2.8 (3)
C8—O1—C9—C10	−177.15 (15)	O2—C7—C8—O1	3.6 (3)
O4—N1—C3—C2	174.8 (3)	C6—C7—C8—O1	−176.59 (15)
O4—N1—C3—C4	−5.1 (4)	O1—C9—C10—C11	170.13 (17)
O5—N1—C3—C2	−5.4 (3)	O1—C9—C10—C15	−13.2 (3)
O5—N1—C3—C4	174.7 (3)	O3—C9—C10—C11	−12.5 (3)
C6—C1—C2—C3	−0.2 (3)	O3—C9—C10—C15	164.3 (2)
C2—C1—C6—C5	0.4 (3)	C9—C10—C11—Cl1	−6.6 (3)
C2—C1—C6—C7	−178.83 (17)	C9—C10—C11—C12	175.2 (2)
C1—C2—C3—N1	179.79 (19)	C15—C10—C11—Cl1	176.60 (17)
C1—C2—C3—C4	−0.4 (3)	C15—C10—C11—C12	−1.6 (3)
N1—C3—C4—C5	−179.5 (2)	C9—C10—C15—C14	−175.3 (2)
C2—C3—C4—C5	0.7 (4)	C11—C10—C15—C14	1.6 (3)
C3—C4—C5—C6	−0.5 (4)	Cl1—C11—C12—C13	−178.1 (2)
C4—C5—C6—C1	0.0 (3)	C10—C11—C12—C13	0.2 (3)
C4—C5—C6—C7	179.2 (2)	C11—C12—C13—C14	1.3 (4)
C1—C6—C7—O2	−3.7 (3)	C12—C13—C14—C15	−1.3 (4)
C1—C6—C7—C8	176.42 (17)	C13—C14—C15—C10	−0.2 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O3[i]	0.93	2.54	3.258 (2)	135
C8—H8*A*···O3[ii]	0.97	2.59	3.553 (3)	171
C13—H13···Cl1[iii]	0.93	2.82	3.670 (3)	153
C14—H14···O4[i]	0.93	2.50	3.211 (4)	134

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2; (iii) −*x*, *y*+1/2, −*z*+3/2.