

(2,4-Dichlorophenyl)(3-hydroxypiperidin-1-yl)-methanone: crystal structure and Hirshfeld analysis

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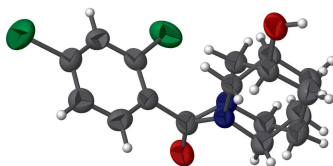
Keywords: crystal structure; piperidine; Hirshfeld surface; two-dimensional fingerprint plot; hydrogen bonding.

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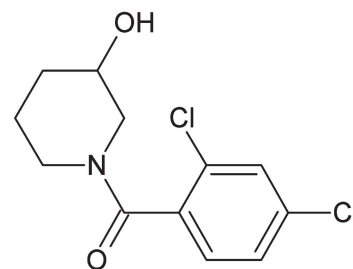
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, C₁₂H₁₃Cl₂NO₂, the piperidine ring adopts a chair conformation. The dihedral angle between the mean plane of the piperidine ring and the benzene ring is 58.5 (3)°. In the crystal, molecules are linked by O—H···O hydrogen bonds, forming chains propagating along the *b*-axis direction. The chains are linked by C—H···O hydrogen bonds, forming undulating sheets parallel to the *ab* plane. The C atoms of the hydroxypiperidine ring are disordered over two sets of sites with refined occupancies of 0.545 (7) and 0.455 (7). The intermolecular interactions in the crystal structure were quantified using Hirshfeld surface analysis.

3D view



Chemical scheme



Structure description

Piperidine derivatives exhibit a wide range of biological activities, such as antimicrobial, anti-inflammatory, antiviral, antimalarial and general anesthetics (Aridoss *et al.*, 2009). The piperidine scaffold has played an important role in numerous pharmaceutical drugs (Das & Brahmachari, 2013). The substitution of hydroxyl, methoxy, nitro and alkyl group on the piperidine ring has been found to produce good antioxidant activities (Ravindernath & Reddy, 2017). Piperidines have also been found to have blood cholesterol-lowering activities (Parthiban *et al.*, 2009). Compounds containing a piperidine moiety are used clinically to prevent post-operative vomiting, to speed up gastric emptying before anaesthesia, to facilitate radiological investigations and to correct a variety of disturbances of gastrointestinal functions (Sampath *et al.*, 2004). Biologically active alkaloids of substituted piperidines have been targeted for their total or partial synthesis (Ramalingan *et al.*, 2004).

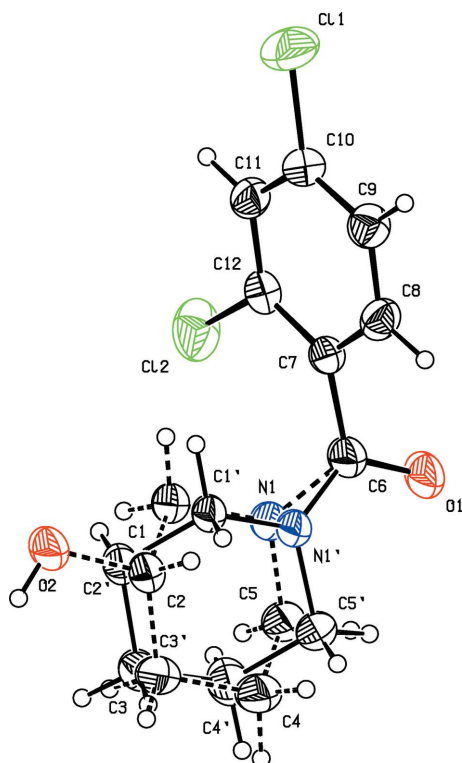


Figure 1
The molecular structure of the title compound, with the atom labelling and displacement ellipsoids drawn at the 30% probability level. The minor component of the piperidine ring has atoms labels N1/C1–C5 and dashed bonds.

The molecular structure of the title compound is illustrated in Fig. 1. The minor component of the piperidine ring has atoms labels N1/C1–C5. The bond lengths and bond angles are

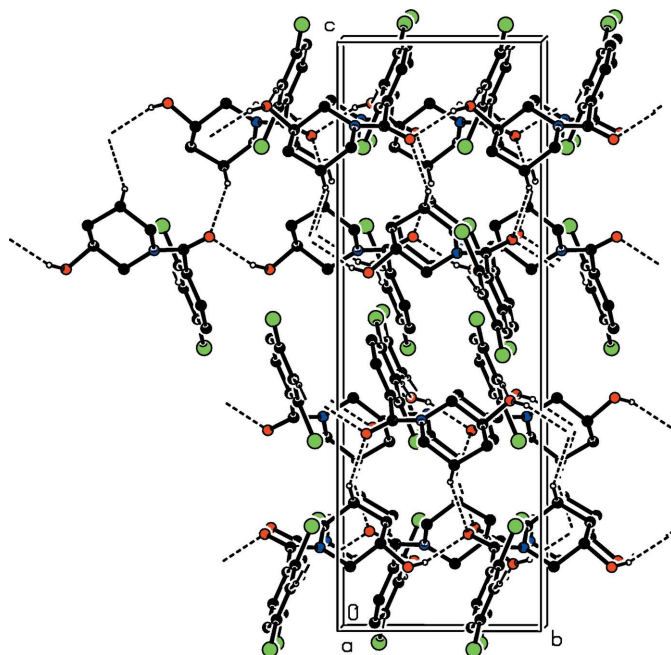


Figure 2
The crystal packing of the title compound, viewed along the *a* axis. The dashed lines indicate the hydrogen bonds (see Table 1). For clarity, only the H atoms involved in these interactions have been included.

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O2–H2A···O1 ⁱ	0.82	2.04	2.735 (3)	142
C11–H11···O2 ⁱⁱ	0.93	2.48	3.404 (4)	173
C4'–H4'1···O1 ⁱⁱⁱ	0.97	2.57	3.456 (12)	152

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

in normal ranges and in good agreement with the values reported for (4-chlorophenyl) 4-hydroxypiperidin-1-yl) methanone (4-chlorophenyl)-(piperidin-1-yl)methanone (0.75/0.25) (Revathi *et al.*, 2015). The dihedral angle between the benzene ring (C7–C12) and the piperidine ring (N1'/C1'–C5') mean plane is 58.5 (3)°. The torsion angle O1–C6–N1'–C5' [12.1 (7)°], indicates that the keto group is in a +*syn*-periplanar (+*sp*) orientation with the hydroxypiperidine ring. The piperidine ring (N1'/C1'–C5') adopts a chair conformation [puckering parameters: $Q = 0.530$ (9) Å, $\theta = 177.5$ (10)° and $\varphi = 351$ (24)°].

In the crystal, molecules are linked by O–H···O hydrogen bonds, forming chains propagating along the *b*-axis direction (Table 1 and Fig. 2). The chains are linked *via* C–H···O hydrogen bonds, forming undulating sheets parallel to the *ab* plane (Table 1 and Fig. 2).

The Hirshfeld analysis (*Crystal Explorer*; Wolff *et al.*, 2012) of the short contacts in the crystal can be summarized with finger print plots mapped over d_{norm} , electrostatic potential,

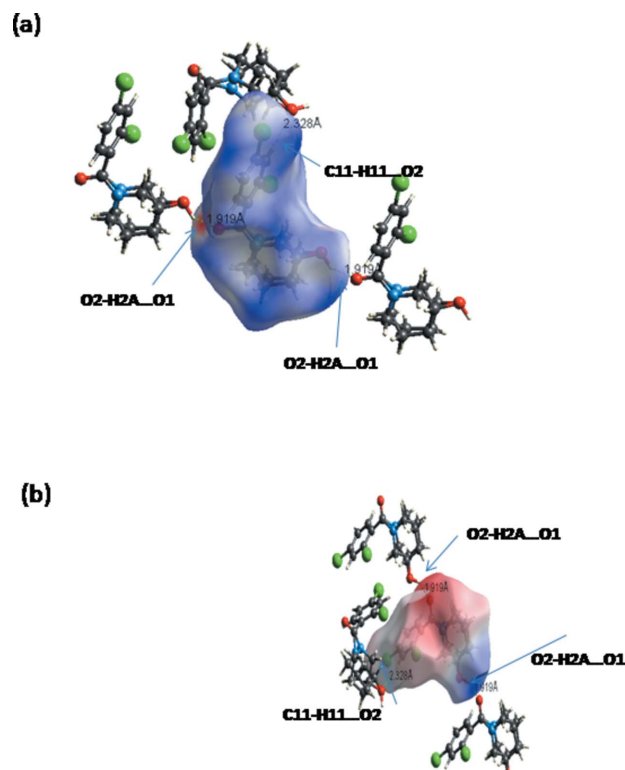


Figure 3
(a) d_{norm} mapped on Hirshfeld surface for visualizing the intermolecular contacts of the title compound. (b) Hirshfeld surfaces mapped over the electrostatic potential. Dotted lines represent hydrogen bonds.

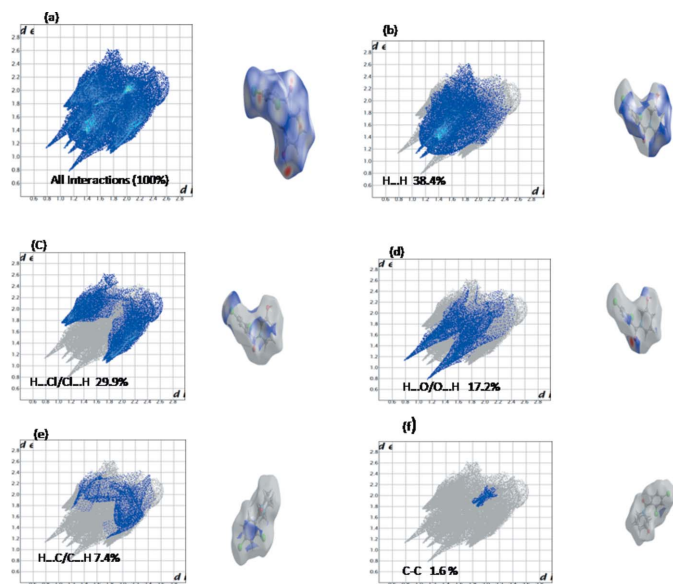


Figure 4

Two-dimensional fingerprint plots of the title compound showing the percentage contributions of individual types of interactions: (a) all intermolecular interactions, (b) H...H contacts, (c) H...Cl/Cl...H contacts and (d) O...H/H...O contacts and (e) H...C/C...H contacts. The outline of the full fingerprint is shown in gray. d_i (x axis) and d_e (y axis) are the closest internal and external distance from a given point on the Hirshfeld surface. Surfaces to the right highlight the relevant surface patches associated with the specific contacts with d_{norm} mapped.

shape index and curvedness. The electrostatic potentials were calculated using *TONTO* (Spackman & Jayatilaka, 2009) integrated within *Crystal Explorer*. The electrostatic potentials were mapped on Hirshfeld surfaces using the STO-3 G basis.

The strong O—H...O and C—H...O interactions are visualized as bright-red spots between the respective donor and acceptor atoms on the Hirshfeld surfaces mapped over d_{norm} (Fig. 3a) with neighbouring molecules connected by O2—H2A...O1 and C11—H11...O2 hydrogen bonds. This observation is revealed in the Hirshfeld surfaces mapped over the electrostatic potential (Fig. 3b) showing the negative potential around the oxygen atoms (light-red clouds) and the positive potential around hydrogen atoms (light-blue clouds). Fingerprint plots (Fig. 4a–f) for the Hirshfeld surfaces of the compound are shown with characteristic pseudo-symmetry wings in the upper left and lower right sides of d_e and d_i diagonal axes that represent the overall two-dimensional fingerprint plot and those delineated into H...H, H...Cl/Cl...H, H...O/O...H, H...C/C...H and C...C contacts.

The fingerprint plot of H...H contacts, which represent the largest contribution to the Hirshfeld surfaces (38.4%), are shown as one distinct pattern with a minimum value of $d_e = d_i \approx 1.4$ Å (Fig. 4b). The H...Cl/Cl...H interactions appear as the next largest region of the fingerprint plot, highly concentrated at the edges, having almost the same $d_e + d_i \approx 2.8$ Å (Fig. 4c), with overall Hirshfeld surfaces of 29.9%. The reciprocal H...O/O...H contacts consists of 17.2% of the total Hirshfeld surfaces with $d_e + d_i \approx 2.0$ Å (Fig. 4d), exhibited by two symmetrical narrow pointed wings indicating the inter-

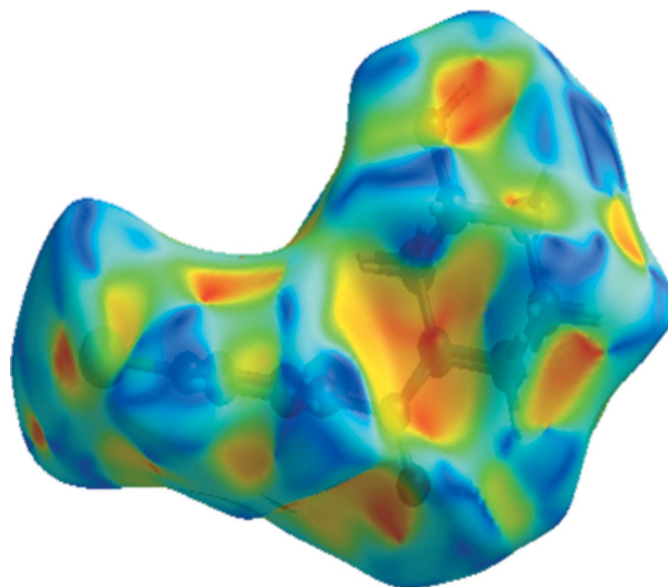


Figure 5

Hirshfeld surfaces mapped over the shape index of the title compound.

molecular hydrogen-bond interactions O2—H2A...O1 and C11—H11...O2 in the crystal packing. The H...C/C...H interaction on the fingerprint plot, which contributes 7.4% of the overall Hirshfeld surfaces, are indicated by $d_e + d_i \approx 3.0$ Å (Fig. 4e). The C...C contacts, which are the measure of π - π stacking interactions, occupy 1.6% of the Hirshfeld surfaces and appear as a unique triangle at about $d_e + d_i \approx 3.8$ Å (Fig. 4f). The existence of π - π interactions is also visualized as red and blue triangles on the shape-indexed surfaces (Fig. 5), and as flat regions on the Hirshfeld surfaces mapped over curvedness in Fig. 6.

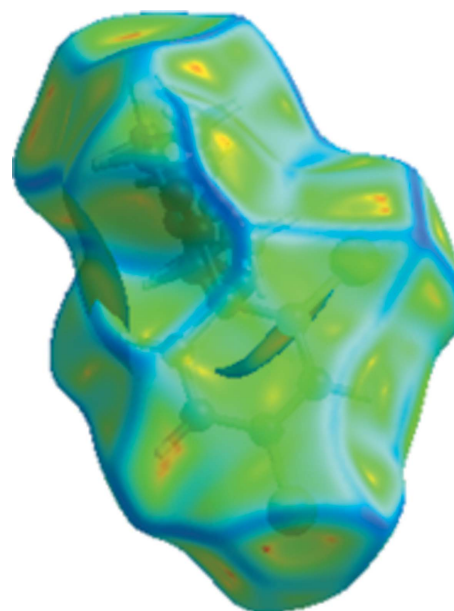


Figure 6

Hirshfeld surfaces mapped over the curvedness of the title compound.

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₂ H ₁₃ Cl ₂ NO ₂
<i>M_r</i>	274.13
Crystal system, space group	Orthorhombic, <i>Pbca</i>
Temperature (K)	298
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.9866 (6), 7.9972 (4), 23.122 (1)
<i>V</i> (Å ³)	2586.3 (2)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
<i>μ</i> (mm ⁻¹)	0.49
Crystal size (mm)	0.35 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2004)
<i>T_{min}</i> , <i>T_{max}</i>	0.892, 0.945
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	34472, 2763, 1602
<i>R_{int}</i>	0.046
(sin θ/λ) _{max} (Å ⁻¹)	0.635
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.048, 0.164, 1.05
No. of reflections	2763
No. of parameters	210
No. of restraints	99
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.26, -0.37

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Synthesis and crystallization

The title compound was synthesized following a published procedure (Revathi *et al.*, (2015)). In a 250 ml round-bottomed flask, 100 ml of ethyl methyl ketone was added to 3-hydroxy piperidine (0.02 mol) and stirred at room temperature. After 5 min, triethylamine (0.04 mol) was added and the mixture was stirred for 15 min. Then 2,4-dichloro benzoyl chloride (0.04 mol) was added and the reaction mixture was stirred at room temperature for 2 h. A white precipitate of triethyl ammonium chloride was formed, which was removed by filtration and the filtrate was evaporated to give the crude

product. It was recrystallized twice from ethyl methyl ketone to give yellow block-like crystals of the title compound (yield: 80%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C atoms of the hydroxy-piperidine ring were refined as disordered, over two set of sites with refined occupancies of 0.545 (7) (N1'/C1'-C5') and 0.455 (7) [N1/C1-C5]. Distance restraints SADI, RIGU and DFIX were used to restrain bond lengths to target values.

Acknowledgements

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full crystallographic data

IUCrData (2017). 2, x170813 [https://doi.org/10.1107/S2414314617008136]

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(2,4-Dichlorophenyl)(3-hydroxypiperidin-1-yl)methanone

Crystal data

$C_{12}H_{13}Cl_2NO_2$

$M_r = 274.13$

Orthorhombic, *Pbca*

$a = 13.9866$ (6) Å

$b = 7.9972$ (4) Å

$c = 23.122$ (1) Å

$V = 2586.3$ (2) Å³

$Z = 8$

$F(000) = 1136$

$D_x = 1.408$ Mg m⁻³

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

Cell parameters from 7296 reflections

$\theta = 2.3$ – 22.7°

$\mu = 0.49$ mm⁻¹

$T = 298$ K

Block, yellow

$0.35 \times 0.25 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

ω and ϕ scan

Absorption correction: multi-scan
(SADABS; Bruker, 2004)

$T_{\min} = 0.892$, $T_{\max} = 0.945$

34472 measured reflections

2763 independent reflections

1602 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 26.9^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -15 \rightarrow 17$

$k = -10 \rightarrow 10$

$l = -25 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.164$

$S = 1.05$

2763 reflections

210 parameters

99 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

$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 1.3359P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.26$ e Å⁻³

$\Delta\rho_{\min} = -0.37$ e Å⁻³

Extinction correction: SHELXL2014
(Sheldrick, 2015),

$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0031 (8)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
N1	0.5092 (5)	0.0739 (7)	0.6677 (3)	0.0590 (18)	0.455 (7)
C1	0.4668 (5)	-0.0842 (8)	0.6489 (3)	0.060 (2)	0.455 (7)
H1A	0.4179	-0.0624	0.6201	0.071*	0.455 (7)
H1B	0.4367	-0.1387	0.6817	0.071*	0.455 (7)
C2	0.5422 (6)	-0.1979 (9)	0.6237 (4)	0.0564 (19)	0.455 (7)
H2	0.5683	-0.1471	0.5885	0.068*	0.455 (7)
C3	0.6208 (9)	-0.2243 (19)	0.6662 (6)	0.067 (3)	0.455 (7)
H3A	0.6706	-0.2914	0.6485	0.081*	0.455 (7)
H3B	0.5963	-0.2856	0.6992	0.081*	0.455 (7)
C4	0.6630 (7)	-0.0618 (12)	0.6866 (5)	0.073 (2)	0.455 (7)
H4A	0.6956	-0.0077	0.6546	0.087*	0.455 (7)
H4B	0.7098	-0.0838	0.7166	0.087*	0.455 (7)
C5	0.5869 (6)	0.0530 (11)	0.7098 (4)	0.066 (2)	0.455 (7)
H5A	0.5614	0.0071	0.7454	0.079*	0.455 (7)
H5B	0.6149	0.1611	0.7185	0.079*	0.455 (7)
N1'	0.5416 (4)	0.0869 (6)	0.6416 (3)	0.0533 (13)	0.545 (7)
C1'	0.5157 (4)	-0.0624 (6)	0.6095 (2)	0.0505 (15)	0.545 (7)
H1'1	0.5635	-0.0836	0.5800	0.061*	0.545 (7)
H1'2	0.4548	-0.0445	0.5903	0.061*	0.545 (7)
C2'	0.5083 (5)	-0.2121 (7)	0.6488 (3)	0.0543 (16)	0.545 (7)
H2'	0.4530	-0.1992	0.6744	0.065*	0.545 (7)
C3'	0.5973 (8)	-0.2377 (16)	0.6844 (5)	0.072 (3)	0.545 (7)
H3'1	0.6500	-0.2688	0.6593	0.086*	0.545 (7)
H3'2	0.5871	-0.3277	0.7118	0.086*	0.545 (7)
C4'	0.6221 (8)	-0.0775 (10)	0.7167 (4)	0.087 (2)	0.545 (7)
H4'1	0.5736	-0.0565	0.7459	0.104*	0.545 (7)
H4'2	0.6827	-0.0922	0.7365	0.104*	0.545 (7)
C5'	0.6287 (5)	0.0717 (8)	0.6773 (4)	0.0698 (19)	0.545 (7)
H5'1	0.6370	0.1723	0.7002	0.084*	0.545 (7)
H5'2	0.6840	0.0600	0.6523	0.084*	0.545 (7)
Cl2	0.28658 (9)	0.11880 (14)	0.68040 (4)	0.0990 (4)	
Cl1	0.17370 (7)	0.32088 (17)	0.47207 (5)	0.1185 (5)	
O2	0.49103 (16)	-0.3471 (2)	0.60880 (9)	0.0738 (7)	
H2A	0.5240	-0.4291	0.6164	0.111*	
O1	0.52333 (18)	0.3567 (3)	0.66457 (10)	0.0819 (7)	
C11	0.2423 (2)	0.2233 (4)	0.57471 (12)	0.0592 (7)	
H11	0.1798	0.1935	0.5839	0.071*	
C12	0.3156 (2)	0.2009 (3)	0.61377 (12)	0.0557 (7)	
C8	0.4269 (2)	0.3131 (4)	0.54690 (12)	0.0578 (7)	

H8	0.4889	0.3446	0.5375	0.069*
C7	0.40901 (18)	0.2434 (3)	0.60078 (12)	0.0516 (7)
C10	0.2645 (2)	0.2910 (4)	0.52185 (12)	0.0618 (8)
C6	0.4908 (2)	0.2295 (4)	0.64243 (13)	0.0647 (8)
C9	0.3554 (2)	0.3364 (4)	0.50740 (13)	0.0617 (8)
H9	0.3686	0.3824	0.4713	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.062 (4)	0.042 (2)	0.073 (4)	−0.002 (2)	−0.022 (3)	−0.002 (2)
C1	0.059 (3)	0.044 (3)	0.075 (4)	−0.003 (2)	−0.014 (3)	−0.002 (3)
C2	0.062 (4)	0.041 (4)	0.066 (4)	−0.002 (3)	−0.010 (3)	0.004 (3)
C3	0.062 (5)	0.060 (5)	0.080 (6)	0.009 (4)	−0.015 (4)	0.001 (4)
C4	0.069 (4)	0.066 (4)	0.084 (5)	0.004 (3)	−0.028 (4)	0.000 (4)
C5	0.068 (4)	0.058 (4)	0.072 (4)	−0.002 (3)	−0.024 (3)	0.000 (3)
N1′	0.058 (3)	0.041 (2)	0.061 (3)	−0.0049 (17)	−0.016 (2)	0.0019 (19)
C1′	0.055 (3)	0.040 (2)	0.057 (3)	−0.004 (2)	−0.012 (2)	0.0009 (19)
C2′	0.065 (4)	0.042 (3)	0.056 (3)	−0.007 (3)	−0.010 (2)	0.002 (2)
C3′	0.083 (5)	0.054 (3)	0.080 (6)	−0.010 (3)	−0.032 (4)	0.015 (4)
C4′	0.112 (6)	0.064 (4)	0.083 (4)	−0.017 (4)	−0.046 (4)	0.011 (3)
C5′	0.067 (3)	0.059 (4)	0.083 (4)	−0.008 (3)	−0.030 (3)	0.005 (3)
C12	0.1290 (9)	0.0990 (8)	0.0690 (6)	−0.0346 (6)	0.0016 (5)	0.0209 (5)
C11	0.0863 (7)	0.1429 (11)	0.1263 (9)	−0.0206 (6)	−0.0527 (6)	0.0448 (7)
O2	0.0858 (15)	0.0407 (11)	0.0950 (16)	0.0020 (10)	−0.0279 (12)	−0.0061 (10)
O1	0.1036 (18)	0.0439 (13)	0.0982 (16)	−0.0080 (11)	−0.0416 (14)	−0.0033 (11)
C11	0.0446 (14)	0.0559 (17)	0.0771 (18)	−0.0014 (13)	0.0041 (14)	0.0004 (15)
C12	0.0639 (18)	0.0435 (15)	0.0598 (16)	−0.0027 (13)	0.0022 (13)	0.0017 (12)
C8	0.0466 (15)	0.0568 (17)	0.0700 (18)	−0.0026 (13)	0.0047 (13)	−0.0064 (14)
C7	0.0511 (16)	0.0369 (14)	0.0668 (17)	0.0017 (12)	−0.0082 (12)	−0.0051 (12)
C10	0.0520 (17)	0.0607 (19)	0.0728 (18)	0.0015 (14)	−0.0097 (14)	0.0044 (15)
C6	0.0714 (19)	0.0430 (15)	0.0797 (19)	−0.0009 (13)	−0.0217 (15)	−0.0021 (14)
C9	0.0645 (18)	0.0639 (19)	0.0568 (16)	−0.0043 (15)	0.0013 (14)	0.0022 (14)

Geometric parameters (Å, °)

N1—C6	1.398 (7)	C2′—C3′	1.507 (11)
N1—C1	1.462 (8)	C2′—H2′	0.9800
N1—C5	1.469 (8)	C3′—C4′	1.524 (13)
C1—C2	1.510 (10)	C3′—H3′1	0.9700
C1—H1A	0.9700	C3′—H3′2	0.9700
C1—H1B	0.9700	C4′—C5′	1.505 (12)
C2—O2	1.434 (8)	C4′—H4′1	0.9700
C2—C3	1.491 (13)	C4′—H4′2	0.9700
C2—H2	0.9800	C5′—H5′1	0.9700
C3—C4	1.503 (15)	C5′—H5′2	0.9700
C3—H3A	0.9700	C12—C12	1.723 (3)
C3—H3B	0.9700	C11—C10	1.731 (3)

C4—C5	1.504 (14)	O2—H2A	0.8200
C4—H4A	0.9700	O1—C6	1.226 (3)
C4—H4B	0.9700	C11—C10	1.372 (4)
C5—H5A	0.9700	C11—C12	1.378 (4)
C5—H5B	0.9700	C11—H11	0.9300
N1'—C6	1.344 (6)	C12—C7	1.383 (4)
N1'—C1'	1.452 (6)	C8—C9	1.367 (4)
N1'—C5'	1.476 (6)	C8—C7	1.387 (4)
C1'—C2'	1.506 (7)	C8—H8	0.9300
C1'—H1'1	0.9700	C7—C6	1.500 (4)
C1'—H1'2	0.9700	C10—C9	1.364 (4)
C2'—O2	1.442 (7)	C9—H9	0.9300
C6—N1—C1	124.8 (5)	O2—C2'—H2'	109.6
C6—N1—C5	121.0 (5)	C1'—C2'—H2'	109.6
C1—N1—C5	113.4 (6)	C3'—C2'—H2'	109.6
N1—C1—C2	110.6 (6)	C2'—C3'—C4'	110.0 (9)
N1—C1—H1A	109.5	C2'—C3'—H3'1	109.7
C2—C1—H1A	109.5	C4'—C3'—H3'1	109.7
N1—C1—H1B	109.5	C2'—C3'—H3'2	109.7
C2—C1—H1B	109.5	C4'—C3'—H3'2	109.7
H1A—C1—H1B	108.1	H3'1—C3'—H3'2	108.2
O2—C2—C3	114.1 (8)	C5'—C4'—C3'	112.5 (7)
O2—C2—C1	104.2 (6)	C5'—C4'—H4'1	109.1
C3—C2—C1	110.2 (8)	C3'—C4'—H4'1	109.1
O2—C2—H2	109.4	C5'—C4'—H4'2	109.1
C3—C2—H2	109.4	C3'—C4'—H4'2	109.1
C1—C2—H2	109.4	H4'1—C4'—H4'2	107.8
C2—C3—C4	111.9 (10)	N1'—C5'—C4'	110.7 (6)
C2—C3—H3A	109.2	N1'—C5'—H5'1	109.5
C4—C3—H3A	109.2	C4'—C5'—H5'1	109.5
C2—C3—H3B	109.2	N1'—C5'—H5'2	109.5
C4—C3—H3B	109.2	C4'—C5'—H5'2	109.5
H3A—C3—H3B	107.9	H5'1—C5'—H5'2	108.1
C3—C4—C5	111.2 (9)	C2—O2—H2A	109.5
C3—C4—H4A	109.4	C10—C11—C12	117.8 (3)
C5—C4—H4A	109.4	C10—C11—H11	121.1
C3—C4—H4B	109.4	C12—C11—H11	121.1
C5—C4—H4B	109.4	C11—C12—C7	121.9 (3)
H4A—C4—H4B	108.0	C11—C12—C12	117.4 (2)
N1—C5—C4	110.8 (7)	C7—C12—C12	120.7 (2)
N1—C5—H5A	109.5	C9—C8—C7	121.6 (3)
C4—C5—H5A	109.5	C9—C8—H8	119.2
N1—C5—H5B	109.5	C7—C8—H8	119.2
C4—C5—H5B	109.5	C12—C7—C8	117.6 (2)
H5A—C5—H5B	108.1	C12—C7—C6	124.3 (3)
C6—N1'—C1'	125.0 (4)	C8—C7—C6	118.0 (3)
C6—N1'—C5'	119.9 (5)	C9—C10—C11	122.3 (3)

C1'—N1'—C5'	115.1 (5)	C9—C10—C11	119.0 (2)
N1'—C1'—C2'	111.3 (4)	C11—C10—C11	118.7 (2)
N1'—C1'—H1'1	109.4	O1—C6—N1'	120.9 (3)
C2'—C1'—H1'1	109.4	O1—C6—N1	119.7 (3)
N1'—C1'—H1'2	109.4	O1—C6—C7	119.3 (3)
C2'—C1'—H1'2	109.4	N1'—C6—C7	117.2 (3)
H1'1—C1'—H1'2	108.0	N1—C6—C7	118.3 (3)
O2—C2'—C1'	102.8 (4)	C10—C9—C8	118.8 (3)
O2—C2'—C3'	112.8 (7)	C10—C9—H9	120.6
C1'—C2'—C3'	112.4 (6)	C8—C9—H9	120.6
C6—N1—C1—C2	113.1 (9)	C11—C12—C7—C6	177.0 (3)
C5—N1—C1—C2	-56.9 (9)	C12—C12—C7—C6	-2.5 (4)
N1—C1—C2—O2	178.6 (5)	C9—C8—C7—C12	-1.2 (4)
N1—C1—C2—C3	55.8 (10)	C9—C8—C7—C6	-177.3 (3)
O2—C2—C3—C4	-172.0 (8)	C12—C11—C10—C9	-0.3 (5)
C1—C2—C3—C4	-55.2 (11)	C12—C11—C10—C11	-179.8 (2)
C2—C3—C4—C5	54.0 (13)	C1'—N1'—C6—O1	-170.7 (4)
C6—N1—C5—C4	-115.2 (10)	C5'—N1'—C6—O1	12.1 (7)
C1—N1—C5—C4	55.3 (10)	C1'—N1'—C6—C7	-8.9 (7)
C3—C4—C5—N1	-52.7 (12)	C5'—N1'—C6—C7	173.9 (5)
C6—N1'—C1'—C2'	-123.6 (7)	C1—N1—C6—O1	173.5 (6)
C5'—N1'—C1'—C2'	53.8 (7)	C5—N1—C6—O1	-17.2 (9)
N1'—C1'—C2'—O2	-175.0 (4)	C1—N1—C6—C7	12.0 (9)
N1'—C1'—C2'—C3'	-53.6 (9)	C5—N1—C6—C7	-178.6 (5)
O2—C2'—C3'—C4'	168.9 (6)	C12—C7—C6—O1	-105.1 (4)
C1'—C2'—C3'—C4'	53.4 (10)	C8—C7—C6—O1	70.7 (4)
C2'—C3'—C4'—C5'	-53.3 (12)	C12—C7—C6—N1'	92.8 (5)
C6—N1'—C5'—C4'	124.2 (9)	C8—C7—C6—N1'	-91.4 (4)
C1'—N1'—C5'—C4'	-53.3 (9)	C12—C7—C6—N1	56.4 (6)
C3'—C4'—C5'—N1'	52.4 (12)	C8—C7—C6—N1	-127.8 (5)
C10—C11—C12—C7	-0.5 (4)	C11—C10—C9—C8	0.2 (5)
C10—C11—C12—C12	179.0 (2)	C11—C10—C9—C8	179.8 (2)
C11—C12—C7—C8	1.2 (4)	C7—C8—C9—C10	0.5 (4)
C12—C12—C7—C8	-178.3 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2 <i>A</i> ...O1 ⁱ	0.82	2.04	2.735 (3)	142
C11—H11...O2 ⁱⁱ	0.93	2.48	3.404 (4)	173
C4'—H4'1...O1 ⁱⁱⁱ	0.97	2.57	3.456 (12)	152

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