



Crystal structure of the adduct (4-chlorophenyl)(4-hydroxypiperidin-1-yl)methanone–(4-chlorophenyl)- (piperidin-1-yl)methanone (0.75/0.25)

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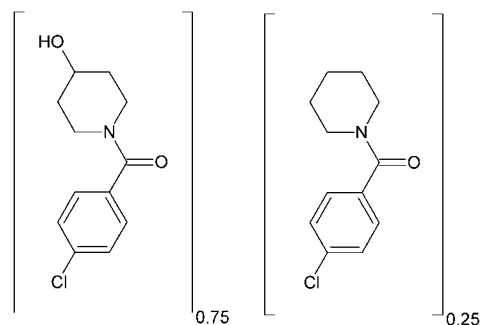
In the title compound, 0.75C₁₂H₁₄ClNO₂·0.25C₁₂H₁₄ClNO, which is an adduct comprising 0.75 4-hydroxypiperidin-1-yl or 0.25 4-piperidin-1-yl substituents on a common (4-chlorophenyl)methanone component; the dihedral angles between the benzene ring and the two piperidine rings are 51.6 (3) and 89.5 (7)°, respectively. The hydroxypiperidine ring is in a bisectonal orientation (*bi*) with the phenyl ring. In the crystal, intermolecular O—H...O hydrogen bonds between the hydroxypiperidine group and the keto O atom lead to the formation of chains extending along the *c*-axis direction.

Keywords: crystal structure; adduct; piperidine derivative; hydrogen bonding.

CCDC reference: 1433393

1. Related literature

For the synthesis, see: Revathi *et al.* (2015). For the biological activity of piperidine derivatives, see: Ramalingan *et al.* (2004); Sargent & May (1970); Rubiralta *et al.* (1991). For related structures, see: Revathi *et al.* (2015); Prathebha *et al.* (2015).



2. Experimental

2.1. Crystal data

0.75C₁₂H₁₄ClNO₂·0.25C₁₂H₁₄ClNO
M_r = 235.69
Orthorhombic, *Pca*2₁
a = 24.312 (4) Å
b = 6.1628 (10) Å
c = 7.9654 (11) Å

V = 1193.5 (3) Å³
Z = 4
Mo *K*α radiation
μ = 0.30 mm⁻¹
T = 293 K
0.25 × 0.20 × 0.20 mm

2.2. Data collection

Bruker Kappa APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2004)
T_{min} = 0.930, *T_{max}* = 0.941

17321 measured reflections
2356 independent reflections
1539 reflections with *I* > 2σ(*I*)
R_{int} = 0.031

2.3. Refinement

R [*F*² > 2σ(*F*²)] = 0.048
wR (*F*²) = 0.144
S = 1.02
2356 reflections
200 parameters
121 restraints
H-atom parameters constrained
Δ*ρ_{max}* = 0.31 e Å⁻³

Δ*ρ_{min}* = -0.22 e Å⁻³
Absolute structure: Flack *x*
determined using 583 quotients
[(*I*⁺ − *I*[−])] / [(*I*⁺ + *I*[−])] (Parsons
et al., 2013)
Absolute structure parameter:
0.03 (3)

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 ¹	0.82	2.05	2.693 (7)	135

Symmetry code: (i) *x*, *y*, *z* − 1.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREF* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL2014*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: ZS2348).

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supporting information

Acta Cryst. (2015). E71, o896–o897 [doi:10.1107/S2056989015020265]

Crystal structure of the adduct (4-chlorophenyl)(4-hydroxypiperidin-1-yl)methanone–(4-chlorophenyl)(piperidin-1-yl)methanone (0.75/0.25)

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S1. Comment

Piperidine is very important pharmacophore because of its presence in numerous alkaloids, pharmaceuticals, agrochemicals and as synthetic intermediates. Biologically active alkaloids with substituted piperidine ring systems have been targeted for their total or partial synthesis (Ramalingan *et al.*, 2004). Piperidines are known to have CNS depressant action at low dosage levels and stimulant activity with increased dosages. In addition, the nucleus also possesses analgesic, ganglionic blocking and anesthetic properties as well (Sargent & May, 1970; Rubiralta *et al.*, 1991).

In the title compound, 0.75(C₁₂H₁₄NO₂Cl) · 0.25(C₁₂H₁₄NOCl), which is an adduct comprising 0.75(4-hydroxypiperidin-1-yl) or 0.25(4-piperidin-1-yl) substituents on a common (4-chlorophenyl)methanone component, the dihedral angles between the benzene ring and the two piperidine rings defined by N1–C12 and N1'–C12' are 51.6 (3) and 89.5 (7)°, respectively (Figs. 1, 2). The C–C distances in the hydroxypiperidine ring and the benzene ring are in the range [1.472 (9)–1.529 (8)Å and 1.346 (7)–1.390 (8)Å], respectively and are in good agreement with literature values (Allen *et al.*, 1987). The C–N distances are in the range [1.346 (7)Å - 1.465 (7)Å] and are in good agreement with values in a similar reported structure (Revathi *et al.*, 2015). The C–O distance [1.223 (6)Å] indicates double bond character and is comparable with the value reported previously (Prathebha *et al.*, 2015). The hydroxypiperidine ring is in a bisectonal orientation (*bi*) with the phenyl ring. The sum of the bond angle around the N1 atom is [359.9 (5)°], showing sp² hybridization of the atoms. The torsion angle C8–N1–C7–O1 [12.3 (10)°], indicates that the keto group is in a *+syn-periplanar* (*+sp*) orientation with the hydroxy piperidine ring. The hydroxypiperidine ring adopts a chair conformation with puckering parameters of q₂ = 0.029Å, phi₂ = -173.57° q₃ = -0.555Å, QT = 0.555Å and theta₂ = 176.95°.

In the crystal, molecules are linked by O2–H···O1ⁱ hydrogen bonds (Table 1), forming one-dimensional chains extending along *c* (Fig. 3). Present also are very weak inter-chain C12'–H···C11ⁱⁱ interactions [3.63 (2) Å]. For symmetry code (ii) $-x + 3/2, -y + 1, z - 1$.

S2. Experimental

The title compound was synthesized by utilizing a reported procedure (Revathi *et al.*, 2015). In a 250 ml round-bottomed flask, 130 ml of ethylmethylketone was added to 4-hydroxypiperidene (0.04 mol) and stirred well. Triethylamine (0.04 mol) was then added and the mixture was stirred for 10 min. 4-Chlorobenzoyl chloride (0.04 mol) was added and the reaction mixture was stirred at room temperature for about 2 hr. A white precipitate of triethylammonium chloride was produced, which was filtered and the filtrate was evaporated to obtain the crude product, crystallization from ethylmethylketone gave colourless block-like crystals of the unexpected title adduct (yield: 88%).

S3. Refinement

H atoms were positioned geometrically and treated as riding on their parent atoms and refined with, C—H distances of 0.93–0.98 Å, an O—H distance of 0.82 Å, with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C-methyl})$, $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C,O})$ for other H atoms. The value of the absolute structure parameter (Parsons *et al.*, 2013), although of no relevance for the present structure was determined as 0.03 (3) using 583 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$.

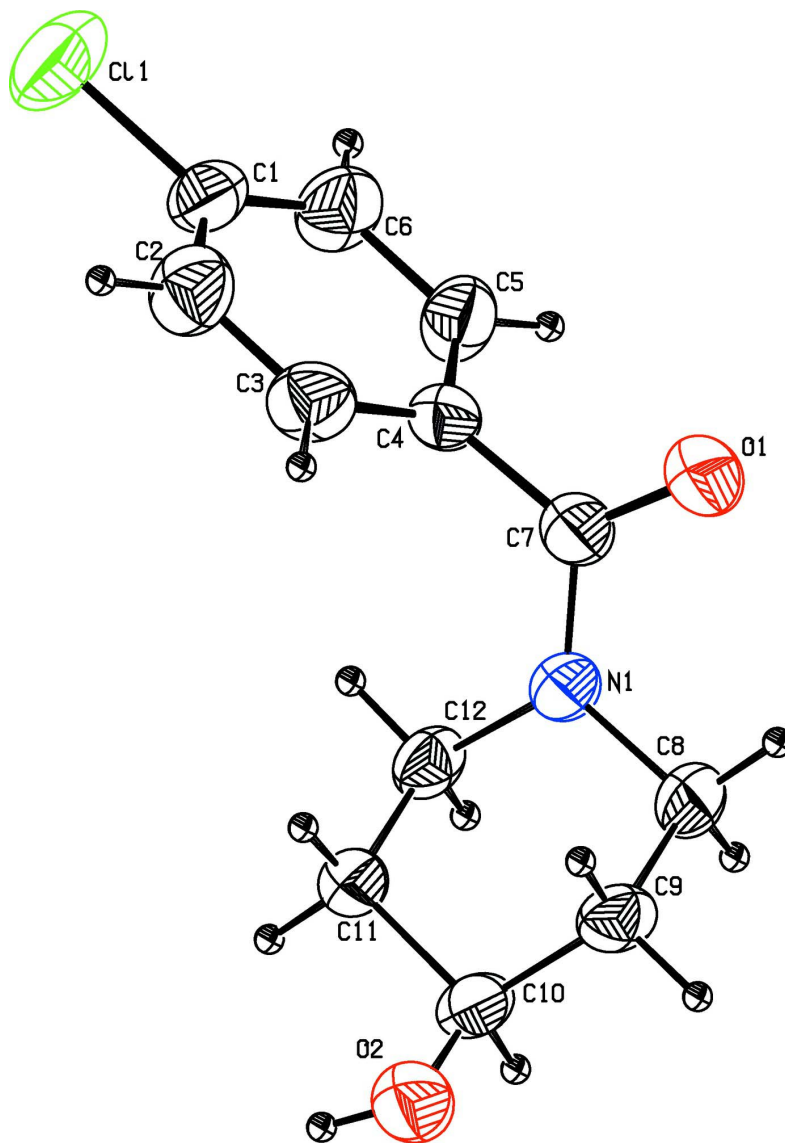


Figure 1

The molecular structure of the major (73%) 4-hydroxypiperidin-1-yl substituted component of the title adduct, showing atom numbering, with displacement ellipsoids drawn at the 30% probability level.

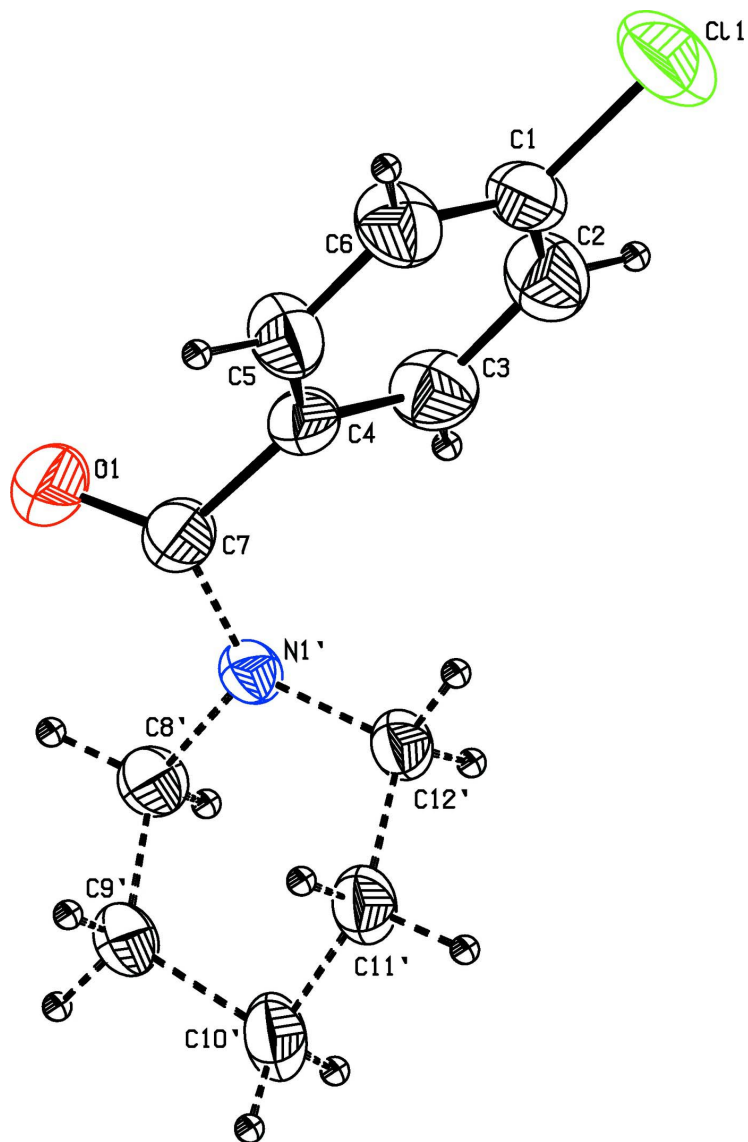


Figure 2

The molecular structure of the minor (25%) piperidin-1-yl substituted component of the title adduct, showing atom numbering, with displacement ellipsoids drawn at the 30% probability level. The bonds for the minor-occupancy piperidinyl group are shown as dashed lines

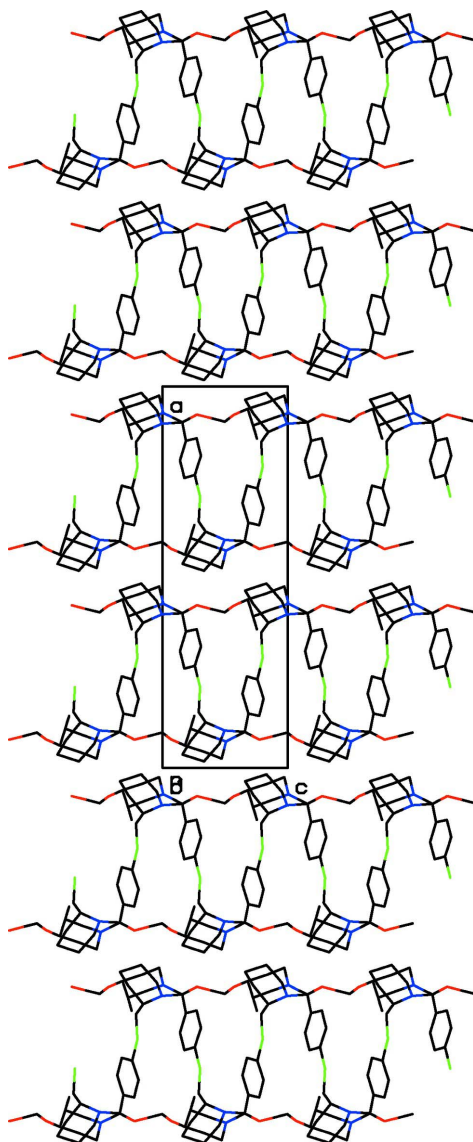


Figure 3

The packing of the molecules in the crystal structure. The dashed lines indicate the O—H...O hydrogen bonds and weak inter-chain C—H...Cl interactions.

(4-Chlorophenyl)(4-hydroxypiperidin-1-yl)methanone–(4-chlorophenyl)(piperidin-1-yl)methanone (0.75/0.25)

Crystal data

$0.75\text{C}_{12}\text{H}_{14}\text{ClNO}_2 \cdot 0.25\text{C}_{12}\text{H}_{14}\text{ClNO}$

$M_r = 235.69$

Orthorhombic, $Pca2_1$

$a = 24.312 (4) \text{ \AA}$

$b = 6.1628 (10) \text{ \AA}$

$c = 7.9654 (11) \text{ \AA}$

$V = 1193.5 (3) \text{ \AA}^3$

$Z = 4$

$F(000) = 496$

$D_x = 1.312 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3452 reflections

$\theta = 2.8\text{--}23.2^\circ$

$\mu = 0.30 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

$0.25 \times 0.20 \times 0.20 \text{ mm}$

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: Sealed tube

ω and φ scan

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

$T_{\min} = 0.930$, $T_{\max} = 0.941$

17321 measured reflections

2356 independent reflections

1539 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 26.1^\circ$, $\theta_{\min} = 3.1^\circ$

$h = -30 \rightarrow 30$

$k = -7 \rightarrow 7$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.144$

$S = 1.02$

2356 reflections

200 parameters

121 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

$w = 1/[\sigma^2(F_o^2) + (0.0664P)^2 + 0.3379P]$

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

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

$\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$

Absolute structure: Flack x determined using
583 quotients $[(F^-)-(F)]/[(F^+)+(F)]$ (Parsons *et al.*,
2013)

Absolute structure parameter: 0.03 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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)
C1	0.73230 (19)	0.1884 (8)	0.7580 (6)	0.0743 (13)	
C2	0.7397 (2)	0.3762 (10)	0.6747 (8)	0.0909 (16)	
H2	0.7748	0.4191	0.6416	0.109*	
C3	0.6943 (2)	0.5050 (9)	0.6390 (7)	0.0832 (15)	
H3	0.6991	0.6353	0.5819	0.100*	
C4	0.64254 (19)	0.4423 (8)	0.6867 (5)	0.0656 (12)	
C5	0.63637 (19)	0.2510 (8)	0.7729 (8)	0.0811 (14)	
H5	0.6016	0.2076	0.8082	0.097*	
C6	0.6815 (2)	0.1230 (8)	0.8074 (8)	0.0890 (16)	
H6	0.6771	-0.0076	0.8643	0.107*	
C7	0.5944 (2)	0.5838 (9)	0.6575 (6)	0.0773 (14)	
C8	0.5243 (3)	0.7357 (12)	0.4730 (9)	0.0749 (18)	0.75
H8A	0.5155	0.8165	0.5739	0.090*	0.75
H8B	0.4918	0.6565	0.4381	0.090*	0.75
C9	0.5419 (3)	0.8877 (11)	0.3372 (9)	0.0681 (17)	0.75
H9A	0.5727	0.9741	0.3766	0.082*	0.75
H9B	0.5119	0.9855	0.3109	0.082*	0.75
C10	0.5587 (3)	0.7668 (13)	0.1804 (9)	0.0711 (19)	0.75

H10	0.5263	0.6897	0.1375	0.085*	0.75
C11	0.6028 (3)	0.5988 (12)	0.2233 (8)	0.0690 (16)	0.75
H11A	0.6102	0.5109	0.1249	0.083*	0.75
H11B	0.6365	0.6732	0.2537	0.083*	0.75
C12	0.5859 (3)	0.4567 (10)	0.3627 (8)	0.0640 (14)	0.75
H12A	0.5554	0.3660	0.3269	0.077*	0.75
H12B	0.6162	0.3627	0.3935	0.077*	0.75
N1	0.5694 (2)	0.5841 (9)	0.5067 (6)	0.0659 (14)	0.75
O2	0.5746 (2)	0.8993 (9)	0.0685 (7)	0.0870 (14)	0.75
H2A	0.5924	0.8339	-0.0030	0.105 (17)*	0.75
C8'	0.5628 (8)	0.863 (3)	0.454 (3)	0.069 (4)	0.25
H8'1	0.5850	0.9758	0.4031	0.083*	0.25
H8'2	0.5466	0.9203	0.5556	0.083*	0.25
C9'	0.5169 (8)	0.795 (4)	0.331 (2)	0.072 (5)	0.25
H9'1	0.4939	0.9210	0.3107	0.087*	0.25
H9'2	0.4942	0.6872	0.3865	0.087*	0.25
C10'	0.5350 (9)	0.703 (4)	0.160 (2)	0.077 (6)	0.25
H10A	0.5559	0.8073	0.0953	0.093*	0.25
H10B	0.5040	0.6510	0.0946	0.093*	0.25
C11'	0.5714 (8)	0.515 (3)	0.226 (3)	0.069 (5)	0.25
H11C	0.5475	0.4128	0.2838	0.082*	0.25
H11D	0.5864	0.4396	0.1295	0.082*	0.25
C12'	0.6196 (7)	0.568 (3)	0.345 (2)	0.057 (4)	0.25
H12C	0.6383	0.4350	0.3775	0.069*	0.25
H12D	0.6458	0.6610	0.2887	0.069*	0.25
N1'	0.5977 (6)	0.677 (2)	0.4953 (15)	0.053 (3)	0.25
O1	0.57385 (17)	0.6828 (7)	0.7749 (5)	0.1119 (14)	
Cl1	0.78823 (7)	0.0274 (3)	0.7998 (3)	0.1274 (8)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.067 (3)	0.080 (3)	0.076 (3)	0.011 (2)	-0.016 (2)	-0.004 (3)
C2	0.070 (3)	0.098 (4)	0.104 (4)	-0.010 (3)	0.001 (3)	0.003 (4)
C3	0.091 (4)	0.076 (3)	0.083 (4)	-0.003 (3)	-0.002 (3)	0.018 (3)
C4	0.073 (3)	0.071 (3)	0.053 (2)	0.012 (2)	0.002 (2)	0.010 (2)
C5	0.066 (3)	0.080 (3)	0.097 (3)	0.007 (3)	0.011 (3)	0.019 (3)
C6	0.092 (4)	0.072 (3)	0.103 (4)	0.017 (3)	0.001 (3)	0.023 (3)
C7	0.090 (3)	0.082 (3)	0.061 (2)	0.029 (3)	0.005 (2)	0.006 (2)
C8	0.074 (4)	0.076 (4)	0.075 (4)	0.031 (3)	0.005 (3)	0.011 (3)
C9	0.080 (5)	0.057 (3)	0.068 (4)	0.018 (3)	-0.012 (3)	0.004 (3)
C10	0.067 (4)	0.081 (4)	0.066 (3)	0.020 (3)	-0.018 (3)	-0.003 (3)
C11	0.067 (4)	0.082 (4)	0.058 (4)	0.020 (3)	-0.004 (3)	-0.004 (3)
C12	0.063 (3)	0.056 (3)	0.074 (3)	0.017 (3)	-0.010 (3)	-0.008 (3)
N1	0.072 (3)	0.064 (3)	0.062 (3)	0.023 (3)	-0.001 (2)	0.006 (2)
O2	0.097 (4)	0.088 (3)	0.076 (3)	0.017 (3)	0.004 (3)	0.004 (3)
C8'	0.079 (9)	0.064 (8)	0.064 (9)	0.032 (7)	-0.003 (8)	-0.001 (6)
C9'	0.067 (9)	0.080 (12)	0.071 (9)	0.034 (8)	-0.001 (7)	-0.007 (9)

C10'	0.057 (11)	0.085 (12)	0.090 (9)	0.012 (9)	0.012 (7)	-0.020 (8)
C11'	0.054 (8)	0.079 (10)	0.073 (9)	0.006 (7)	0.002 (7)	-0.023 (7)
C12'	0.050 (7)	0.059 (9)	0.062 (7)	0.009 (7)	0.001 (6)	-0.008 (6)
N1'	0.051 (7)	0.052 (6)	0.055 (4)	0.012 (5)	-0.004 (4)	-0.004 (4)
O1	0.121 (3)	0.147 (3)	0.067 (2)	0.057 (3)	0.008 (2)	-0.004 (3)
Cl1	0.0952 (10)	0.1290 (13)	0.1579 (17)	0.0462 (9)	-0.0304 (12)	-0.0134 (14)

Geometric parameters (Å, °)

C1—C2	1.346 (7)	C10—H10	0.9800
C1—C6	1.358 (7)	C11—C12	1.472 (9)
C1—Cl1	1.716 (5)	C11—H11A	0.9700
C2—C3	1.390 (8)	C11—H11B	0.9700
C2—H2	0.9300	C12—N1	1.447 (8)
C3—C4	1.370 (7)	C12—H12A	0.9700
C3—H3	0.9300	C12—H12B	0.9700
C4—C5	1.373 (7)	O2—H2A	0.8200
C4—C7	1.478 (7)	C8'—N1'	1.460 (16)
C5—C6	1.378 (6)	C8'—C9'	1.54 (2)
C5—H5	0.9300	C8'—H8'1	0.9700
C6—H6	0.9300	C8'—H8'2	0.9700
C7—O1	1.223 (6)	C9'—C10'	1.540 (12)
C7—N1	1.346 (7)	C9'—H9'1	0.9700
C7—N1'	1.417 (13)	C9'—H9'2	0.9700
C8—N1	1.465 (7)	C10'—C11'	1.552 (12)
C8—C9	1.494 (9)	C10'—H10A	0.9700
C8—H8A	0.9700	C10'—H10B	0.9700
C8—H8B	0.9700	C11'—C12'	1.542 (19)
C9—C10	1.510 (9)	C11'—H11C	0.9700
C9—H9A	0.9700	C11'—H11D	0.9700
C9—H9B	0.9700	C12'—N1'	1.474 (16)
C10—O2	1.269 (9)	C12'—H12C	0.9700
C10—C11	1.529 (8)	C12'—H12D	0.9700
C2—C1—C6	121.4 (5)	C10—C11—H11B	109.2
C2—C1—Cl1	119.1 (4)	H11A—C11—H11B	107.9
C6—C1—Cl1	119.5 (4)	N1—C12—C11	110.6 (5)
C1—C2—C3	119.0 (5)	N1—C12—H12A	109.5
C1—C2—H2	120.5	C11—C12—H12A	109.5
C3—C2—H2	120.5	N1—C12—H12B	109.5
C4—C3—C2	120.8 (5)	C11—C12—H12B	109.5
C4—C3—H3	119.6	H12A—C12—H12B	108.1
C2—C3—H3	119.6	C7—N1—C12	125.6 (5)
C3—C4—C5	118.8 (4)	C7—N1—C8	120.2 (5)
C3—C4—C7	121.1 (4)	C12—N1—C8	114.1 (5)
C5—C4—C7	119.9 (4)	C10—O2—H2A	109.5
C4—C5—C6	120.3 (5)	N1'—C8'—C9'	110.8 (15)
C4—C5—H5	119.9	N1'—C8'—H8'1	109.5

C6—C5—H5	119.9	C9'—C8'—H8'1	109.5
C1—C6—C5	119.7 (5)	N1'—C8'—H8'2	109.5
C1—C6—H6	120.1	C9'—C8'—H8'2	109.5
C5—C6—H6	120.1	H8'1—C8'—H8'2	108.1
O1—C7—N1	119.8 (5)	C8'—C9'—C10'	116.9 (17)
O1—C7—N1'	121.2 (6)	C8'—C9'—H9'1	108.1
O1—C7—C4	119.8 (4)	C10'—C9'—H9'1	108.1
N1—C7—C4	119.9 (5)	C8'—C9'—H9'2	108.1
N1'—C7—C4	109.8 (6)	C10'—C9'—H9'2	108.1
N1—C8—C9	108.5 (6)	H9'1—C9'—H9'2	107.3
N1—C8—H8A	110.0	C9'—C10'—C11'	98.0 (15)
C9—C8—H8A	110.0	C9'—C10'—H10A	112.2
N1—C8—H8B	110.0	C11'—C10'—H10A	112.2
C9—C8—H8B	110.0	C9'—C10'—H10B	112.2
H8A—C8—H8B	108.4	C11'—C10'—H10B	112.2
C8—C9—C10	111.5 (6)	H10A—C10'—H10B	109.8
C8—C9—H9A	109.3	C12'—C11'—C10'	118.9 (17)
C10—C9—H9A	109.3	C12'—C11'—H11C	107.6
C8—C9—H9B	109.3	C10'—C11'—H11C	107.6
C10—C9—H9B	109.3	C12'—C11'—H11D	107.6
H9A—C9—H9B	108.0	C10'—C11'—H11D	107.6
O2—C10—C9	110.2 (6)	H11C—C11'—H11D	107.0
O2—C10—C11	112.2 (6)	N1'—C12'—C11'	108.7 (13)
C9—C10—C11	109.8 (5)	N1'—C12'—H12C	109.9
O2—C10—H10	108.2	C11'—C12'—H12C	109.9
C9—C10—H10	108.2	N1'—C12'—H12D	109.9
C11—C10—H10	108.2	C11'—C12'—H12D	109.9
C12—C11—C10	112.0 (6)	H12C—C12'—H12D	108.3
C12—C11—H11A	109.2	C7—N1'—C8'	119.5 (12)
C10—C11—H11A	109.2	C7—N1'—C12'	125.0 (12)
C12—C11—H11B	109.2	C8'—N1'—C12'	112.7 (13)
C6—C1—C2—C3	0.0 (8)	C10—C11—C12—N1	-53.4 (9)
C11—C1—C2—C3	179.1 (5)	O1—C7—N1—C12	-173.2 (6)
C1—C2—C3—C4	-0.3 (8)	C4—C7—N1—C12	-1.0 (10)
C2—C3—C4—C5	0.9 (8)	O1—C7—N1—C8	12.3 (10)
C2—C3—C4—C7	176.6 (5)	C4—C7—N1—C8	-175.4 (6)
C3—C4—C5—C6	-1.3 (8)	C11—C12—N1—C7	-116.7 (7)
C7—C4—C5—C6	-177.0 (5)	C11—C12—N1—C8	58.0 (9)
C2—C1—C6—C5	-0.3 (9)	C9—C8—N1—C7	115.9 (7)
C11—C1—C6—C5	-179.5 (5)	C9—C8—N1—C12	-59.2 (9)
C4—C5—C6—C1	1.0 (9)	N1'—C8'—C9'—C10'	-60 (3)
C3—C4—C7—O1	-104.8 (7)	C8'—C9'—C10'—C11'	56 (2)
C5—C4—C7—O1	70.8 (7)	C9'—C10'—C11'—C12'	-57 (2)
C3—C4—C7—N1	82.9 (7)	C10'—C11'—C12'—N1'	59 (2)
C5—C4—C7—N1	-101.4 (6)	O1—C7—N1'—C8'	-18.1 (18)
C3—C4—C7—N1'	42.4 (9)	C4—C7—N1'—C8'	-164.8 (13)
C5—C4—C7—N1'	-142.0 (8)	O1—C7—N1'—C12'	-177.3 (12)

N1—C8—C9—C10	56.9 (9)	C4—C7—N1'—C12'	36.0 (17)
C8—C9—C10—O2	-178.5 (7)	C9'—C8'—N1'—C7	-108.1 (19)
C8—C9—C10—C11	-54.4 (9)	C9'—C8'—N1'—C12'	54 (2)
O2—C10—C11—C12	175.3 (7)	C11'—C12'—N1'—C7	108.5 (19)
C9—C10—C11—C12	52.4 (9)	C11'—C12'—N1'—C8'	-52 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O2—H2 <i>A</i> \cdots O1 ⁱ	0.82	2.05	2.693 (7)	135
C12'—H12 <i>D</i> \cdots C11 ⁱⁱ	0.97	2.77	3.63 (2)	148

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