Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of (4-chlorophenyl)(4-methylpiperidin-1-yl)methanone

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Received 27 January 2020
Accepted 10 February 2020

Edited by J. Jasinsk, Keene State College, USA

Keywords: crystal structure; piperidine; piperidin-1-yl; Hirshfeld surface.

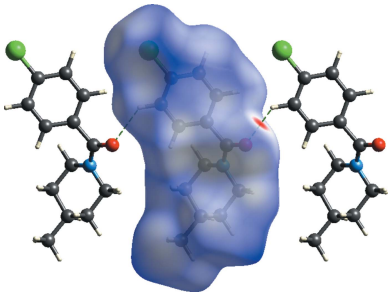
CCDC reference: 1973841

Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, $C_{13}H_{16}ClNO$, contains a methylpiperidine ring in the stable chair conformation. The mean plane of the twisted piperidine ring subtends a dihedral angle of 39.89 (7)° with that of the benzene ring. In the crystal, weak C—H···O interactions link the molecules along the *a*-axis direction to form infinite molecular chains. H···H interatomic interactions, C—H···O intermolecular interactions and weak dispersive forces stabilize molecular packing and form a supramolecular network, as established by Hirshfeld surface analysis.

1. Chemical context

The structures of a wide variety of heterocyclic derivatives have been analysed for their pharma-potentiality over the past three decades (Katritzky, 2010). Among them, derivatives of the six-membered heterocyclic base piperidine have proven to be successful pharmacophores. Naturally existing in abundance, alkaloids of substituted piperidine compounds exhibit a wide range of biological activities (Yunusov & Azimova, 2013). Anti-convulsant (Santucci *et al.*, 1986), anti-tumor, anti-bacterial (Vinaya *et al.*, 2009), anti-viral (Abdel-Aziza *et al.*, 2010), anti-fungal (Rafiq *et al.*, 2013) and plasma triglyceride-lowering (Uto *et al.*, 2010) activities, along with their antagonist activity as anti-HIV-1 agents (Imamura *et al.*, 2005) are deserving of mention. Piperidin-1-yl derivatives have proven vital in the field of neuropsychosis due to their potent biological activity. They act as either central nervous system (CNS) depressants or as stimuli, based on dosage levels (Ramalingan *et al.*, 2004), and also show anti-tubercular (Patel *et al.*, 2011), anti-cancer (Lefranc *et al.*, 2013), anti-tumor (da Silveira *et al.*, 2017) and, in particular, anti-leukemic (Vinaya *et al.*, 2011) activities. One such active piperidin-1-yl derivative is the title compound, (4-chlorophenyl)(4-methyl piperidin-1-yl)methanone.



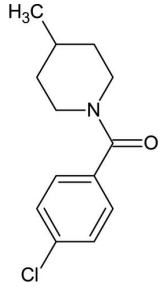


Table 1
Hydrogen-bond geometry (Å, °).

*Cg*2 is the centroid of the C7–C12 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.93	2.46	3.166 (3)	132
C2—H2*A*···*Cg*2^{ii}	0.97	2.95	3.843 (3)	154

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

2. Structural commentary

The molecular structure of the title compound, which features a chlorobenzene ring and a methylpiperidine ring, is shown in Fig. 1. The C—N distances [1.343 (3)–1.462 (3) Å], C═O distance [1.233 (3) Å] and all other primary bond lengths along with bond angles are well within the range reported for similar structures (Prathebha *et al.*, 2015). The ring puckering parameters [q_2 = 0.005 (3), q_3 = −0.551 (3), Q_T = 0.551 (3) Å, φ_2 = 203 (32)° and θ = 180.0 (3)°] confirm that the piperidine ring adopts a chair conformation. The C1—N1—C6—O1 and O1—C6—C7—C8 torsion angles are −167.4 (2) and 50.7 (3)°, respectively. The C1—C2—C3—C13 torsion angle [177.7 (2)°] reveals the anti-periplanar (+ap) orientation of the methyl group with respect to the piperidine ring.

3. Supramolecular features

In the crystal, weak C11—H11···O1 interactions link translation-related molecules ($x-1, y, z$), forming chains parallel to the *a* axis (Table 1, Fig. 2*a*). Weak C—H···π close contacts between H5*A* and the benzene ring of an adjacent ($1-x, -y, -z$) molecule provide linkage between inversion-related (*i.e.*, head-to-tail) chains (Table 1, Fig. 2*b*). Analysis of the Hirshfeld surface (Spackman *et al.*, 2009) and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were performed with *CrystalExplorer 17* (Turner *et al.*, 2017). Hirshfeld surfaces mapped over d_{norm}, were generated using *TONTO* (Jayatilaka *et al.*, 2005) computations with B3LYP/6-31G(d,p) basis sets (Fig. 3). Among the major non-bonding interactions (Fig. 4), H···H contacts have the highest percentage contribution of 52.1%, followed by Cl···H/H···Cl (18.8%), C···H/H···C (16.3%), O···H/H···O (10.4%) and C···O/O···C (1.1%) interactions. The electrostatic and the polarization energies observed among the molecules are compensated by the repulsive components, while the C—H···O interactions along with van der Waals dispersive forces contribute to form the supramolecular network.

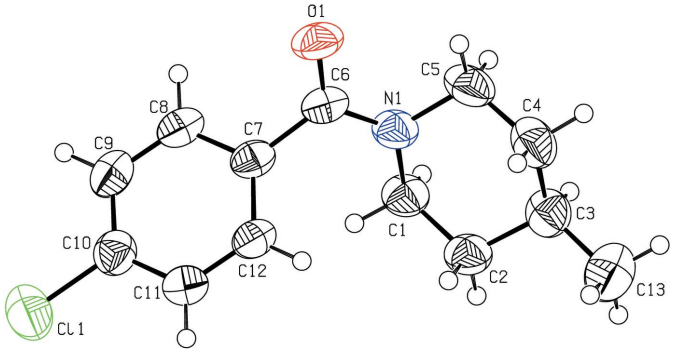


Figure 1
The molecular structure of the title compound showing the atom-labelling scheme with displacement ellipsoids drawn at the 30% probability level.

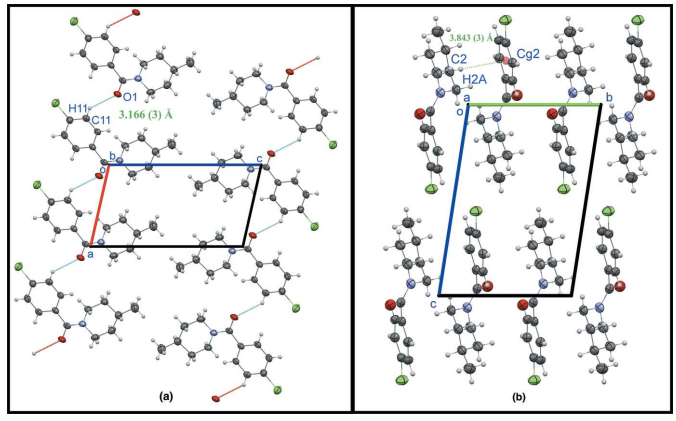


Figure 2
(*a*) The molecular packing viewed perpendicular to the *ac* plane, showing the formation of chains along the *a* axis. Dotted lines indicate weak C—H···O interactions. (*b*) The crystal packing viewed along the *a* axis, showing the weak C—H···π close contacts (green dotted line).

4. Database survey

The Cambridge Structural Database (version 5.40, Nov. 2018; Groom *et al.*, 2016) includes various structural analogues of substituted piperidin-1-yl compounds, which include EYIXIT (Schmittel *et al.*, 2004), AFETUB (Rao *et al.*, 2007), IJUZAP (Betz *et al.*, 2011), NIPCAS (Prathebha *et al.*, 2013), QUTGOD (Revathi *et al.*, 2015*c*), NUKDUU (Revathi *et al.*, 2015*d*), BEBFEW (Mohamooda Sumaya *et al.*, 2017),

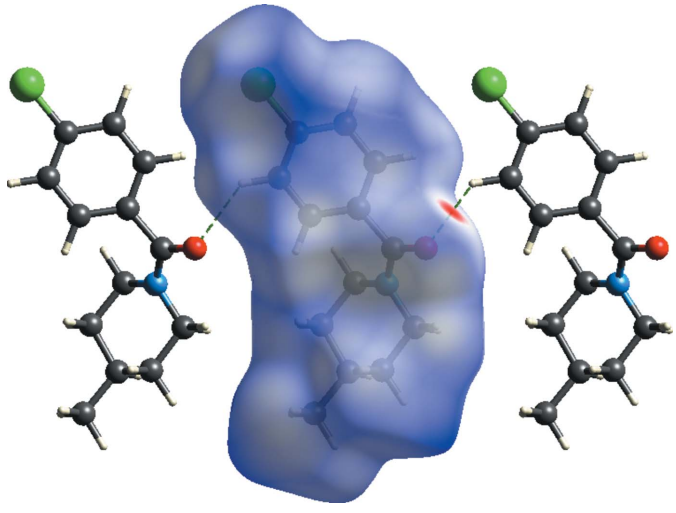


Figure 3
Hirshfeld surfaces mapped over d_{norm} showing weak C—H···O interactions on either side of the molecule.

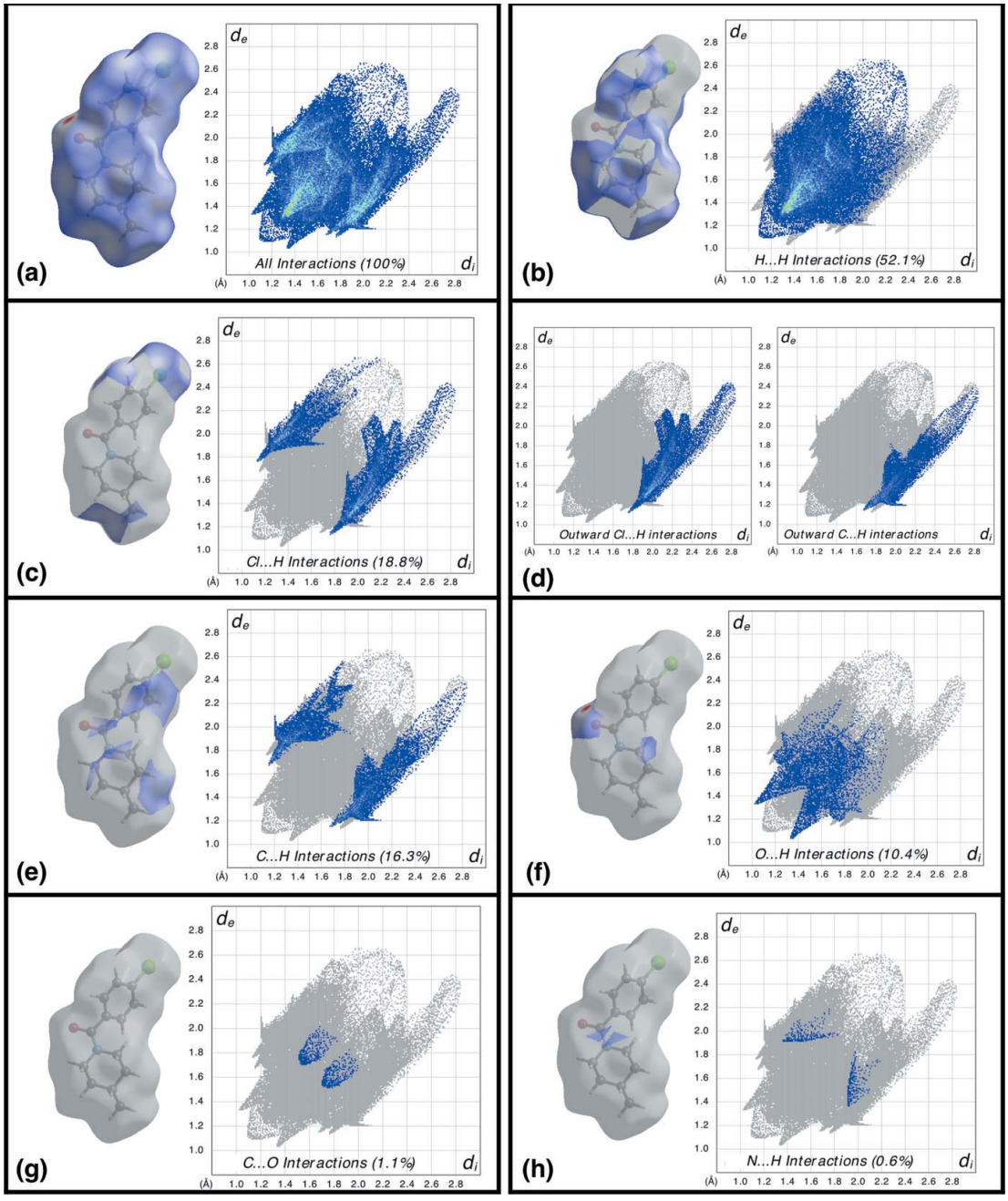


Figure 4
Two-dimensional fingerprint plots illustrating the percentage contributions of contacts within the crystal: (*a*) all intermolecular interactions, (*b*) H···H contacts, (*c*) H···Cl/Cl···H contacts, (*d*) Outward Cl···H and C···H interactions, (*e*) H···C/C···H contacts, (*f*) O···H/H···O contacts, (*g*) C···O/O···C contacts and (*h*) N···H/H···N contacts. The Hirshfeld surfaces mapped over d_{norm} are displayed in grey, with the relevant surface patches associated with the specific contacts highlighted in colour.

GUVXAY (Revathi *et al.*, 2015*a*) and LUPDUX (Revathi *et al.*, 2015*b*).

5. Synthesis and crystallization

The title compound was synthesized using the published procedure (Revathi *et al.*, 2018) *via* a Scholten–Boumann condensation reaction (Fig. 5). A homogeneous mixture of the reagent, 4-methylpiperidine (0.04mol) was prepared with 150ml of methyl ethyl ketone in a round-bottomed flask by stirring it at room temperature for a few minutes. Then 0.04mol of triethylamine was added, followed by stirring for 20min. An equal amount of 2-chlorobenzoyl chloride (0.04mol) was then added slowly under constant stirring and the mixture was then refluxed for 3h at room temperature. The precipitate of triethylammonium chloride formed was filtered off and the filtrate was allowed to evaporate to obtain the title compound. The product was then recrystallized three times from chloroform to obtain block-like single crystals of the title compound, m.p. 325K.

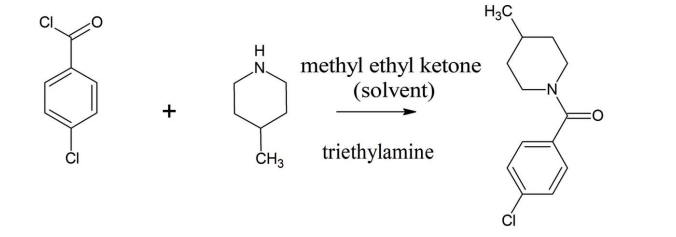


Figure 5
Reaction scheme.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.5U_{eq}(C-methyl) or 1.2U_{eq}(C) for all other H atoms.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{16}ClNO$
M_r	237.72
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	6.6286 (4), 8.1569 (5), 12.0061 (8)
α, β, γ (°)	96.803 (3), 101.506 (3), 98.511 (3)
V (Å^3)	621.73 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	0.25 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker Kappa-axis
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.840, 0.842
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11137, 2178, 1687
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.144, 1.05
No. of reflections	2178
No. of parameters	147
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.25

Computer programs: *APEX3*, *SAINT* and *XPREP* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Acknowledgements

The authors thank the Central Instrumentation Facility, DST–FIST, Queen Mary's College, Chennai-4, for the computing facilities and SAIF, IIT, Madras, for the X-ray data collection.

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supporting information

Acta Cryst. (2020). E**76**, 534-538 [https://doi.org/10.1107/S2056989020001930]

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Computing details

Data collection: *APEX3* (Bruker, 2012); cell refinement: *APEX3*/*SAINT* (Bruker, 2012); data reduction: *SAINT*/*XPREP* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015\bbr06); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(4-Chlorophenyl)(4-methylpiperidin-1-yl)methanone

Crystal data

$C_{13}H_{16}ClNO$
$M_r = 237.72$
Triclinic, $P\overline{1}$
$a = 6.6286$ (4) Å
$b = 8.1569$ (5) Å
$c = 12.0061$ (8) Å
$\alpha = 96.803$ (3)°
$\beta = 101.506$ (3)°
$\gamma = 98.511$ (3)°
$V = 621.73$ (7) Å^3
$Z = 2$
$F(000) = 252$
$D_x = 1.270$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6685 reflections
$\theta = 2.9$–25.1°
$\mu = 0.29$ mm^{-1}
$T = 296$ K
Block, colourless
0.25 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEX3 CMOS diffractometer
Radiation source: fine-focus sealed tube
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
$T_{min} = 0.840$, $T_{max} = 0.842$
11137 measured reflections
2178 independent reflections
1687 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 25.1°$, $\theta_{min} = 3.3°$
$h = -7\rightarrow7$
$k = -9\rightarrow9$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.144$
$S = 1.05$
2178 reflections
147 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
$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.3053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.108 (19)

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.24442 (13)	0.18102 (11)	−0.44227 (6)	0.0859 (4)
O1	1.1366 (2)	0.3558 (2)	−0.04876 (15)	0.0658 (5)
N1	0.9452 (3)	0.2267 (2)	0.06264 (17)	0.0550 (5)
C1	0.7665 (4)	0.1096 (3)	0.0775 (2)	0.0568 (6)
H1A	0.8106	0.0055	0.0947	0.068*
H1B	0.6601	0.0848	0.0065	0.068*
C2	0.6753 (4)	0.1832 (3)	0.1740 (2)	0.0592 (6)
H2A	0.5635	0.1005	0.1858	0.071*
H2B	0.6158	0.2795	0.1523	0.071*
C3	0.8399 (4)	0.2370 (3)	0.2863 (2)	0.0627 (7)
H3	0.8885	0.1362	0.3104	0.075*
C4	1.0257 (4)	0.3522 (4)	0.2649 (2)	0.0699 (8)
H4A	0.9837	0.4571	0.2478	0.084*
H4B	1.1357	0.3770	0.3343	0.084*
C5	1.1111 (4)	0.2761 (4)	0.1664 (2)	0.0672 (7)
H5A	1.2220	0.3572	0.1521	0.081*
H5B	1.1696	0.1787	0.1869	0.081*
C6	0.9693 (3)	0.2802 (3)	−0.0362 (2)	0.0511 (6)
C7	0.7827 (3)	0.2502 (3)	−0.1352 (2)	0.0488 (5)
C8	0.8006 (4)	0.1799 (3)	−0.2430 (2)	0.0557 (6)
H8	0.9259	0.1473	−0.2518	0.067*
C9	0.6368 (4)	0.1573 (3)	−0.3373 (2)	0.0609 (7)
H9	0.6494	0.1071	−0.4087	0.073*
C10	0.4536 (4)	0.2104 (3)	−0.3242 (2)	0.0566 (6)
C11	0.4326 (4)	0.2848 (3)	−0.2191 (2)	0.0551 (6)
H11	0.3092	0.3221	−0.2118	0.066*
C12	0.5960 (3)	0.3036 (3)	−0.1249 (2)	0.0521 (6)
H12	0.5816	0.3525	−0.0535	0.062*
C13	0.7481 (6)	0.3170 (4)	0.3813 (3)	0.0895 (10)
H13A	0.6345	0.2386	0.3935	0.134*
H13B	0.6978	0.4156	0.3593	0.134*
H13C	0.8543	0.3475	0.4511	0.134*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0826 (6)	0.1031 (7)	0.0649 (5)	0.0208 (4)	0.0003 (4)	0.0062 (4)
O1	0.0437 (9)	0.0777 (12)	0.0767 (12)	−0.0028 (8)	0.0272 (8)	0.0079 (9)
N1	0.0407 (10)	0.0592 (12)	0.0636 (12)	−0.0009 (8)	0.0120 (9)	0.0143 (9)
C1	0.0479 (13)	0.0535 (13)	0.0664 (15)	−0.0048 (10)	0.0135 (11)	0.0140 (11)
C2	0.0474 (13)	0.0637 (15)	0.0682 (16)	0.0030 (11)	0.0162 (11)	0.0194 (12)
C3	0.0659 (15)	0.0614 (15)	0.0615 (15)	0.0072 (12)	0.0129 (12)	0.0197 (12)
C4	0.0630 (16)	0.0730 (17)	0.0637 (16)	−0.0050 (13)	−0.0014 (12)	0.0171 (13)
C5	0.0413 (12)	0.0772 (18)	0.0788 (18)	−0.0013 (12)	0.0037 (12)	0.0266 (14)
C6	0.0451 (12)	0.0480 (12)	0.0637 (14)	0.0078 (10)	0.0223 (10)	0.0046 (10)
C7	0.0457 (12)	0.0451 (12)	0.0577 (13)	0.0025 (9)	0.0208 (10)	0.0076 (10)
C8	0.0533 (13)	0.0574 (14)	0.0620 (15)	0.0083 (11)	0.0280 (12)	0.0075 (11)
C9	0.0714 (16)	0.0623 (15)	0.0521 (14)	0.0101 (12)	0.0251 (12)	0.0033 (11)
C10	0.0596 (14)	0.0567 (14)	0.0534 (13)	0.0056 (11)	0.0150 (11)	0.0092 (11)
C11	0.0481 (12)	0.0586 (14)	0.0606 (14)	0.0084 (10)	0.0172 (11)	0.0100 (11)
C12	0.0497 (13)	0.0542 (13)	0.0545 (13)	0.0061 (10)	0.0218 (11)	0.0037 (10)
C13	0.104 (2)	0.094 (2)	0.074 (2)	0.0115 (19)	0.0294 (18)	0.0131 (17)

Geometric parameters (Å, º)

Cl1—C10	1.740 (3)	C5—H5A	0.9700
O1—C6	1.233 (3)	C5—H5B	0.9700
N1—C6	1.343 (3)	C6—C7	1.502 (3)
N1—C5	1.459 (3)	C7—C8	1.388 (3)
N1—C1	1.462 (3)	C7—C12	1.394 (3)
C1—C2	1.513 (3)	C8—C9	1.377 (3)
C1—H1A	0.9700	C8—H8	0.9300
C1—H1B	0.9700	C9—C10	1.379 (4)
C2—C3	1.527 (3)	C9—H9	0.9300
C2—H2A	0.9700	C10—C11	1.376 (3)
C2—H2B	0.9700	C11—C12	1.378 (3)
C3—C4	1.519 (4)	C11—H11	0.9300
C3—C13	1.522 (4)	C12—H12	0.9300
C3—H3	0.9800	C13—H13A	0.9600
C4—C5	1.517 (4)	C13—H13B	0.9600
C4—H4A	0.9700	C13—H13C	0.9600
C4—H4B	0.9700		
C6—N1—C5	120.52 (19)	N1—C5—H5B	109.6
C6—N1—C1	125.8 (2)	C4—C5—H5B	109.6
C5—N1—C1	113.55 (19)	H5A—C5—H5B	108.1
N1—C1—C2	110.72 (19)	O1—C6—N1	123.0 (2)
N1—C1—H1A	109.5	O1—C6—C7	118.5 (2)
C2—C1—H1A	109.5	N1—C6—C7	118.53 (19)
N1—C1—H1B	109.5	C8—C7—C12	118.3 (2)
C2—C1—H1B	109.5	C8—C7—C6	119.34 (19)

H1A—C1—H1B	108.1	C12—C7—C6	122.1 (2)
C1—C2—C3	111.9 (2)	C9—C8—C7	121.4 (2)
C1—C2—H2A	109.2	C9—C8—H8	119.3
C3—C2—H2A	109.2	C7—C8—H8	119.3
C1—C2—H2B	109.2	C8—C9—C10	118.9 (2)
C3—C2—H2B	109.2	C8—C9—H9	120.5
H2A—C2—H2B	107.9	C10—C9—H9	120.5
C4—C3—C13	112.4 (2)	C11—C10—C9	121.2 (2)
C4—C3—C2	109.3 (2)	C11—C10—Cl1	119.38 (19)
C13—C3—C2	111.4 (2)	C9—C10—Cl1	119.45 (19)
C4—C3—H3	107.9	C10—C11—C12	119.4 (2)
C13—C3—H3	107.9	C10—C11—H11	120.3
C2—C3—H3	107.9	C12—C11—H11	120.3
C5—C4—C3	112.6 (2)	C11—C12—C7	120.8 (2)
C5—C4—H4A	109.1	C11—C12—H12	119.6
C3—C4—H4A	109.1	C7—C12—H12	119.6
C5—C4—H4B	109.1	C3—C13—H13A	109.5
C3—C4—H4B	109.1	C3—C13—H13B	109.5
H4A—C4—H4B	107.8	H13A—C13—H13B	109.5
N1—C5—C4	110.3 (2)	C3—C13—H13C	109.5
N1—C5—H5A	109.6	H13A—C13—H13C	109.5
C4—C5—H5A	109.6	H13B—C13—H13C	109.5

C6—N1—C1—C2	−126.7 (2)	O1—C6—C7—C8	50.7 (3)
C5—N1—C1—C2	57.3 (3)	N1—C6—C7—C8	−130.7 (2)
N1—C1—C2—C3	−55.0 (3)	O1—C6—C7—C12	−123.7 (2)
C1—C2—C3—C4	52.9 (3)	N1—C6—C7—C12	54.8 (3)
C1—C2—C3—C13	177.7 (2)	C12—C7—C8—C9	−2.3 (3)
C13—C3—C4—C5	−177.3 (2)	C6—C7—C8—C9	−176.9 (2)
C2—C3—C4—C5	−53.1 (3)	C7—C8—C9—C10	1.8 (4)
C6—N1—C5—C4	126.9 (2)	C8—C9—C10—C11	0.0 (4)
C1—N1—C5—C4	−56.8 (3)	C8—C9—C10—Cl1	−179.41 (19)
C3—C4—C5—N1	54.8 (3)	C9—C10—C11—C12	−1.3 (4)
C5—N1—C6—O1	8.4 (4)	Cl1—C10—C11—C12	178.09 (18)
C1—N1—C6—O1	−167.4 (2)	C10—C11—C12—C7	0.8 (3)
C5—N1—C6—C7	−170.0 (2)	C8—C7—C12—C11	0.9 (3)
C1—N1—C6—C7	14.2 (3)	C6—C7—C12—C11	175.4 (2)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C7–C12 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.93	2.46	3.166 (3)	132
C2—H2*A*···*Cg*2^{ii}	0.97	2.95	3.843 (3)	154

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

The surface property statistics for the generated Hirshfeld Surface

Surface parameter	Min	Mean	Max
d_i (Å)	1.030	1.696	2.851
d_e (Å	1.031	1.699	2.694
d_{norm} (Å)	-0.176	0.537	1.463