research communications

Crystal structure, hydrogen bonding and Hirshfeld surface analysis of 2-amino-4-methoxy-6-methyl-pyrimidinium 4-chlorobenzoate

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In the crystal structure of the title salt, $C_6H_{10}N_3O^+ \cdot C_7H_4ClO_2^-$, the dihedral angle between the pyrimidine ring of the 2-amino-4-methoxy-6-methyl-pyrimidine cation and the the benzene ring of the 2-chlorobenzoate anion is 2.2 (1)°. In the anion, the benzene ring forms a dihedral angle of 8.5 (2)° with the carboxyl group. The pyrimidine N atom of the cation is protonated and the methoxy substituent is essentially coplanar with the parent ring. The protonated N atom and the N atom of the 2-amino group are hydrogen bonded to the 4-chlorobenzoate anion through a pair of $N-H \cdots O_{carboxyl}$ hydrogen bonds, forming an $R_2^2(8)$ ring motif linked through a centrosymmetric $R_4^2(8)$ ring motif, resulting in a pseudotetrameric DDAA array. These units are linked through intermolecular methoxy $C-H \cdots Cl$ hydrogen bonds into ribbon-like chains extending along the c-axis direction. The crystal structure also features $\pi-\pi$ stacking interactions between the rings in the cation and anion [minimum ring centroid separation = 3.7707 (12) Å].

1. Chemical context

Pyrimidine and aminopyrimidine derivatives are biologically important compounds and they occur in nature as components of nucleic acids such as cytosine, uracil and thymine. Pyrimidine derivatives are also important molecules in biology and have many applications in the areas of pesticides and pharmaceutical agents (Condon et al., 1993). For example, imazosulfuron, ethirmol and mepanipyrim have been commercialized as agrochemicals (Maeno et al., 1990). Pyrimidine derivatives have also been developed as antiviral agents, such as AZT, which is the most widely used anti-AIDS drug (Gilchrist, 1997). In order to study the hydrogen-bonding interactions, the title compound, the 2-amino-4-methoxy-6-methylpyrimidinium salt of 4-chlorobenzoate, $C_6H_{10}N_3O^+ \cdot C_7H_4ClO_2^-$, was synthesized and its structure, hydrogen-bonding and Hirshfeld surface analysis are reported herein.
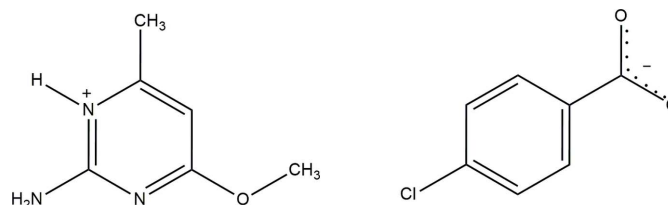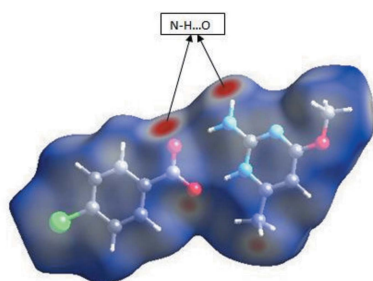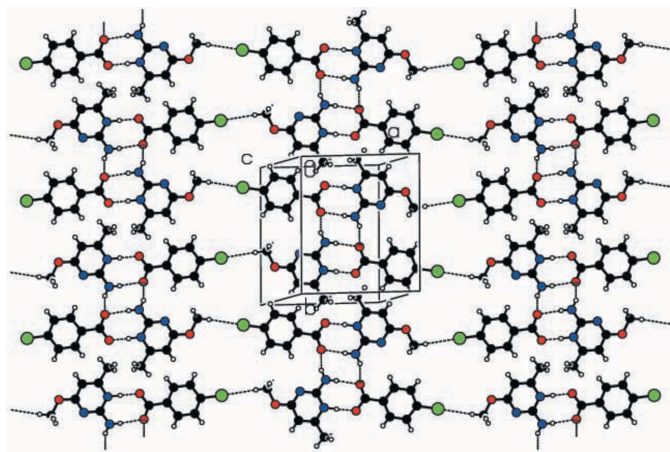

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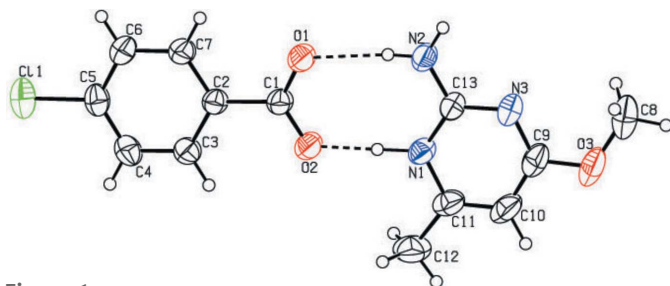
Figure 1
The asymmetric unit of the the title compound with atom labels, showing non-hydrogen atoms as 30% probability displacement ellipsoids. Inter-species hydrogen bonds are shown as dashed lines.

2. Structural commentary

The asymmetric unit of the title compound contains a 2-amino-4-methoxy-6-methylpyrimidinium cation and a 4-chlorobenzoate anion (Fig. 1), which are essentially coplanar, with a dihedral angle between the ring systems of the two species of 2.2 (1)°. In the cation, one of the pyrimidine nitrogen atoms (N1) is protonated and this is reflected in an increase in bond angle at N1 [C11—N1—C13 = 120.53 (17)°], when compared with that at the unprotonated atom (N3) [C9—N3—C13 = 116.32 (18)°] and the corresponding angle of 116.01 (18)° in neutral 2-amino-4-methoxy-6-methyl-pyrimidine (Glidewell *et al.*, 2003). The methoxy substituent group at C9 of the cation is essentially coplanar with the ring, the N3—C9—O3—C8 torsion angle being −2.9 (3)°. The bond lengths and angles are normal for the carboxylate group of a 4-chlorobenzoate anion, and the benzene ring forms a dihedral angle of 8.5 (2)° with the carboxyl group.

3. Supramolecular features

In the crystal, the protonated nitrogen atom (N1) and the amino nitrogen atom (N2) of the cation interact with the carboxyl oxygen atoms O2 and O1, respectively, of the anion through N—H···O hydrogen bonds (Table 1), forming an

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N1···O2	1.04 (3)	1.60 (3)	2.636 (3)	176 (2)
N2—H1N···O1[i]	0.86	2.12	2.846 (2)	142
N2—H2N···O1	0.86	1.97	2.824 (3)	169
C8—H8A···Cl1[ii]	0.96	2.82	3.770 (3)	171

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

eight-membered $R_2^2(8)$ ring motif. This is extended into a *DDAA* array (where *D* represents a hydrogen-bond donor and *A* represents a hydrogen-bond acceptor) by N2—H1N···O1[i] hydrogen bonds in a centrosymmetric $R_4^2(8)$ association [symmetry code: (i) $-x + 1, -y + 2, -z + 1$], the corresponding graph-set notations for the heterotetramer being $R_2^2(8)$, $R_4^2(8)$, $R_2^2(8)$. The heterotetrameric units are linked through methoxy C8—H8A···Cl[ii] hydrogen bonds, forming one-dimensional ribbon-like structures (Fig. 2) [symmetry code: (ii) $x + 2, -y + \frac{3}{2}, z + \frac{1}{2}$]. Only very weak methyl C12—H···O2 interactions [C···O = 3.442 (3) Å; H···O2 = 2.76 Å] exist between ribbons. The crystal structure also features π–π stacking interactions between the aromatic pyrimidine ring of the cation (Fig. 3) and the benzene ring of the anion, with minimum centroid–centroid and perpendicular interplanar distances of 3.7780 (12) and 3.7075 (8) Å, respectively, and a slip angle of 19.44° (Hunter *et al.*, 1994).

4. Hirshfeld surface analysis

Three-dimensional (3D) d_{norm} surface analyis is a useful tool for analysing and visualizing the intermolecular interactions.

Figure 2
Hydrogen bonding in the structure of the title compound showing the $R_2^2(8)$ and centrosymmetric $R_4^2(8)$ ring motifs and C—H···Cl extensions. Dashed lines indicate the hydrogen bonds.
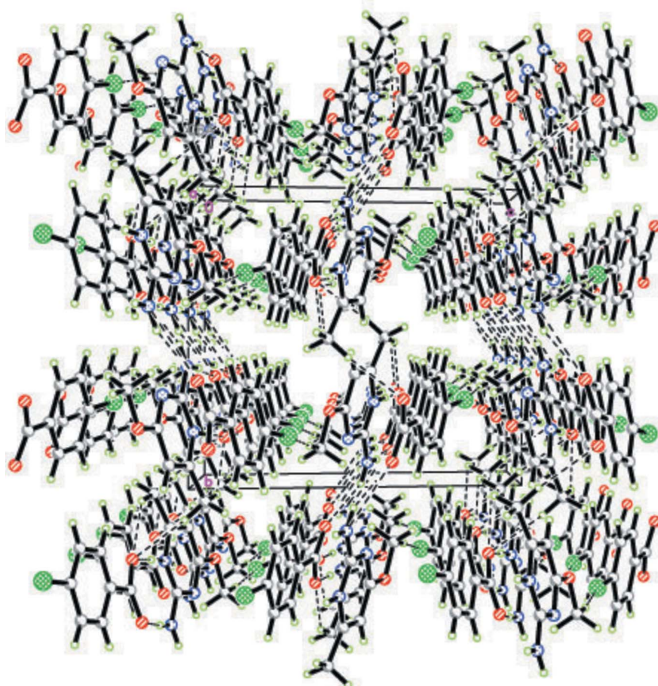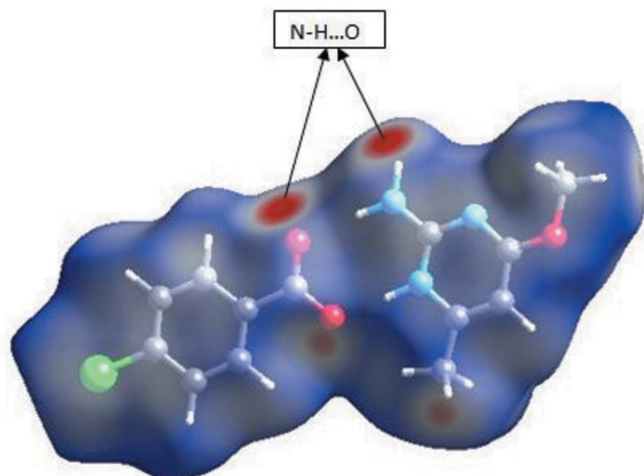

Figure 3
The overall view of the packing and stacking interactions in the title compound.

N–H⋯O

Figure 4
The three-dimensional d_{norm} surface of the title compound.

d_{norm} takes negative or positive values depending on whether the intermolecular contact is shorter or longer, respectively, than the van der Waals radii (Spackman & Jayatilaka, 2009; McKinnon *et al.*, 2007). The 3D d_{norm} surface of the title compound was shown in Fig. 4. The red points represent closer

contacts and negative d_{norm} values on the surface corresponding to the N—H⋯O interactions, while C—H⋯O interactions are light red in colour. Two-dimensional fingerprint plots from the Hirshfeld surface analysis are shown in Fig. 5, revealing the intermolecular contacts and their percentage distributions on the Hirshfeld surface. H⋯H interactions (44.8%) are present as a major contributor while O⋯H/H⋯O (14.6%), H⋯Cl/Cl⋯H (13.3%), C⋯H/H⋯C (7.5%), C⋯C (6.6%), N⋯H/H⋯N (3.4%), C⋯N/N⋯C (3.3%), Cl⋯N/N⋯Cl (1.8%), C⋯Cl/Cl⋯C (1.0%) and Cl⋯O/O⋯Cl (0.7%) contacts also make significant contributions to the Hirshfeld surface. Two 'wingtips' in the fingerprint plot are related to H⋯O and O⋯H interactions and are shown in Fig. 5.

5. Database survey

A search of the Cambridge Structural Database (Version 5.37, update February 2017; Groom *et al.*, 2016) for 2-amino-4-methoxy-6-methylpyrimidine yielded only seven structures of proton-transfer salts with carboxylic acids: VAQSOW [with 3-(*N,N*-dimethylamino)benzoic acid]; VAQSUC [with methylene hydrogen succinic acid (a monohydrate)]; VAQSEM (with 3-nitrobenzoic acid); VAQSIQ (with benzoic acid); VAQRUB (with 2-fluorobenzoic acid) and VAQSAI (with 3-chlorobenzoic acid) (all from Aakeröy *et al.*, 2003) and NUQTOJ (with picric acid; Jasinski *et al.*, 2010).
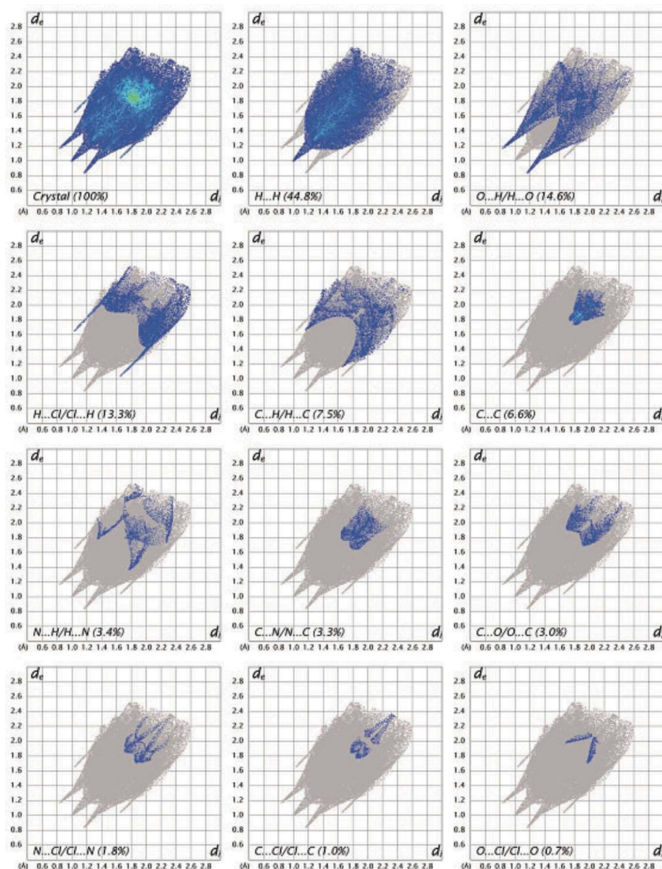
Figure 5
Two-dimensional fingerprint plots with the relative contributions to the Hirshfeld surface.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_{10}N_3O^+\cdot C_7H_4ClO_2^-$
M_r	295.72
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	10.1148 (8), 11.2236 (8), 14.579 (1)
β (°)	120.940 (5)
V (Å^3)	1419.57 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.28
Crystal size (mm)	$0.35 \times 0.30 \times 0.20$
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.909, 0.946
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10962, 3423, 2125
R_{int}	0.024
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.152, 0.99
No. of reflections	3423
No. of parameters	188
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.26, −0.35

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SIR92* (Altomare *et al.*, 1999), *SHELXL2017* (Sheldrick, 2015), *ORTEP-3* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

6. Synthesis and crystallization

The title compound was synthesized by the reaction of a 1:1 stoichiometric mixture of 2-amino-4-methoxy-6-methyl-pyrimidine [0.139 mg (Aldrich)] and 4-chlorobenzoic acid [0.156 mg (Merck)] in 20 ml of a hot methanolic solution. After warming for a few minutes over a water bath, the solution was cooled and kept at room temperature. Within a few days, colourless block-shaped crystals suitable for the X-ray analysis were obtained (yield: 65%).

7. refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. N-bound pyrimidinium H atoms were located in a difference-Fourier map and refined freely [N—H = 1.03 (3) Å]. The remaining H atoms were positioned geometrically and refined using a riding model with (N—H = 0.86 Å and C—H = 0.93 or 0.96 Å) and $U_{iso}(H) = 1.2\ U_{eq}(C,N)$ or $1.5U_{eq}$(methyl C). A rotating-group model was used for the methyl groups.

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Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015); molecular graphics: *ORTEP-3* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2017* (Sheldrick, 2015).

(I)

Crystal data

$C_6H_{10}N_3O^+ \cdot C_7H_4ClO_2^-$	$F(000) = 616$
$M_r = 295.72$	$D_x = 1.384$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 10.1148$ (8) Å	Cell parameters from 3319 reflections
$b = 11.2236$ (8) Å	$\theta = 4.7–53.1°$
$c = 14.579$ (1) Å	$\mu = 0.28$ mm^{-1}
$\beta = 120.940$ (5)°	$T = 296$ K
$V = 1419.57$ (19) Å^3	Block, colorless
$Z = 4$	$0.35 \times 0.30 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	3423 independent reflections
Radiation source: fine-focus sealed tube	2125 reflections with $I > 2\sigma(I)$
ω and φ scan	$R_{int} = 0.024$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$\theta_{max} = 28.4°$, $\theta_{min} = 2.7°$
$T_{min} = 0.909$, $T_{max} = 0.946$	$h = -13 \rightarrow 12$
10962 measured reflections	$k = -14 \rightarrow 14$
	$l = -15 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.047$	Hydrogen site location: mixed
$wR(F^2) = 0.152$	H atoms treated by a mixture of independent and constrained refinement
$S = 0.99$	$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2 + 0.324P]$
3423 reflections	where $P = (F_o^2 + 2F_c^2)/3$
188 parameters	
0 restraints	

$(\Delta/\sigma)_{max} = 0.003$

$\Delta\rho_{max} = 0.26$ e Å^{-3}

$\Delta\rho_{min} = -0.34$ e Å^{-3}

Extinction correction: SHELXL2017
(Sheldrick, 2015),
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.020 (3)

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 (Å^2)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
O3	1.08061 (18)	0.73298 (18)	0.57812 (14)	0.0840 (5)
N1	0.62562 (18)	0.71035 (13)	0.45066 (13)	0.0513 (4)
N2	0.61625 (18)	0.91121 (14)	0.47011 (15)	0.0649 (5)
H1N	0.659761	0.979882	0.489408	0.078*
H2N	0.518251	0.904882	0.442578	0.078*
N3	0.85256 (18)	0.82711 (15)	0.52563 (13)	0.0555 (4)
C8	1.1555 (3)	0.8473 (3)	0.6048 (2)	0.0926 (9)
H8A	1.258389	0.838988	0.618161	0.139*
H8B	1.159254	0.877851	0.667577	0.139*
H8C	1.098704	0.901435	0.546305	0.139*
C9	0.9288 (2)	0.7287 (2)	0.53678 (16)	0.0616 (6)
C10	0.8601 (3)	0.6168 (2)	0.50699 (19)	0.0703 (6)
H10	0.919348	0.548952	0.518504	0.084*
C11	0.7049 (3)	0.60891 (17)	0.46085 (17)	0.0595 (5)
C12	0.6128 (3)	0.49752 (19)	0.4188 (2)	0.0872 (8)
H12A	0.531726	0.509732	0.346014	0.131*
H12B	0.568913	0.477063	0.461457	0.131*
H12C	0.678410	0.433995	0.421663	0.131*
C13	0.6995 (2)	0.81598 (16)	0.48261 (15)	0.0489 (4)
Cl1	−0.42873 (6)	0.70123 (7)	0.18780 (6)	0.0859 (3)
O1	0.30336 (15)	0.87707 (12)	0.40502 (13)	0.0710 (5)
O2	0.32766 (15)	0.68727 (12)	0.37489 (12)	0.0648 (4)
C1	0.2501 (2)	0.77506 (16)	0.37387 (15)	0.0506 (5)
C2	0.0808 (2)	0.75559 (16)	0.33048 (14)	0.0455 (4)
C3	0.0178 (2)	0.64290 (17)	0.30515 (16)	0.0532 (5)
H3	0.081505	0.577740	0.317181	0.064*
C4	−0.1384 (2)	0.62496 (19)	0.26221 (16)	0.0591 (5)
H4	−0.179743	0.548535	0.245653	0.071*
C5	−0.2314 (2)	0.72173 (19)	0.24443 (16)	0.0552 (5)
C6	−0.1725 (2)	0.83473 (19)	0.26959 (17)	0.0615 (5)
H6	−0.237007	0.899426	0.257249	0.074*

C7	−0.0160 (2)	0.85154 (17)	0.31355 (16)	0.0559 (5)
H7	0.025012	0.927932	0.332014	0.067*
H1N1	0.508 (3)	0.700 (2)	0.418 (2)	0.089 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0495 (9)	0.1165 (14)	0.0927 (12)	0.0275 (9)	0.0414 (9)	0.0152 (11)
N1	0.0479 (9)	0.0476 (9)	0.0551 (9)	0.0080 (7)	0.0242 (8)	−0.0032 (7)
N2	0.0389 (8)	0.0483 (9)	0.0946 (13)	0.0010 (7)	0.0251 (8)	−0.0125 (8)
N3	0.0411 (9)	0.0722 (11)	0.0533 (10)	0.0081 (7)	0.0243 (7)	−0.0019 (8)
C8	0.0457 (13)	0.140 (3)	0.0899 (19)	0.0033 (14)	0.0337 (13)	0.0031 (17)
C9	0.0507 (12)	0.0858 (15)	0.0564 (13)	0.0194 (10)	0.0333 (10)	0.0100 (11)
C10	0.0728 (15)	0.0697 (14)	0.0839 (16)	0.0340 (12)	0.0514 (13)	0.0182 (12)
C11	0.0738 (14)	0.0508 (11)	0.0653 (13)	0.0173 (9)	0.0439 (11)	0.0081 (9)
C12	0.112 (2)	0.0478 (12)	0.121 (2)	0.0116 (12)	0.0732 (18)	0.0017 (13)
C13	0.0406 (9)	0.0533 (10)	0.0497 (11)	0.0050 (8)	0.0210 (8)	−0.0029 (8)
Cl1	0.0454 (3)	0.1120 (6)	0.0929 (5)	−0.0142 (3)	0.0302 (3)	−0.0069 (4)
O1	0.0424 (7)	0.0458 (8)	0.1021 (12)	−0.0028 (6)	0.0210 (7)	−0.0149 (7)
O2	0.0454 (8)	0.0481 (7)	0.0872 (11)	0.0023 (6)	0.0242 (7)	−0.0098 (7)
C1	0.0404 (9)	0.0449 (10)	0.0527 (11)	0.0003 (7)	0.0141 (8)	−0.0010 (8)
C2	0.0406 (9)	0.0447 (9)	0.0424 (10)	0.0005 (7)	0.0149 (8)	0.0012 (7)
C3	0.0495 (11)	0.0465 (10)	0.0573 (11)	−0.0031 (8)	0.0230 (9)	−0.0053 (8)
C4	0.0549 (12)	0.0578 (12)	0.0623 (13)	−0.0144 (9)	0.0285 (10)	−0.0095 (10)
C5	0.0416 (10)	0.0722 (13)	0.0468 (11)	−0.0074 (9)	0.0191 (8)	−0.0020 (9)
C6	0.0429 (10)	0.0607 (12)	0.0702 (14)	0.0087 (9)	0.0215 (10)	0.0076 (10)
C7	0.0442 (10)	0.0459 (10)	0.0643 (12)	0.0007 (8)	0.0184 (9)	0.0034 (9)

Geometric parameters (Å, º)

O3—C9	1.331 (2)	C12—H12A	0.9600
O3—C8	1.438 (4)	C12—H12B	0.9600
N1—C13	1.350 (2)	C12—H12C	0.9600
N1—C11	1.356 (2)	Cl1—C5	1.7385 (19)
N1—H1N1	1.03 (3)	O1—C1	1.247 (2)
N2—C13	1.314 (2)	O2—C1	1.255 (2)
N2—H1N	0.8600	C1—C2	1.506 (2)
N2—H2N	0.8600	C2—C3	1.379 (3)
N3—C9	1.308 (3)	C2—C7	1.389 (3)
N3—C13	1.344 (2)	C3—C4	1.383 (3)
C8—H8A	0.9600	C3—H3	0.9300
C8—H8B	0.9600	C4—C5	1.372 (3)
C8—H8C	0.9600	C4—H4	0.9300
C9—C10	1.392 (3)	C5—C6	1.369 (3)
C10—C11	1.356 (3)	C6—C7	1.381 (3)
C10—H10	0.9300	C6—H6	0.9300
C11—C12	1.490 (3)	C7—H7	0.9300

C9—O3—C8	118.61 (18)	H12A—C12—H12C	109.5	
C13—N1—C11	120.53 (17)	H12B—C12—H12C	109.5	
C13—N1—H1N1	124.1 (13)	N2—C13—N3	119.43 (17)	
C11—N1—H1N1	115.4 (13)	N2—C13—N1	117.68 (16)	
C13—N2—H1N	120.0	N3—C13—N1	122.89 (16)	
C13—N2—H2N	120.0	O1—C1—O2	124.51 (17)	
H1N—N2—H2N	120.0	O1—C1—C2	118.10 (16)	
C9—N3—C13	116.32 (18)	O2—C1—C2	117.39 (16)	
O3—C8—H8A	109.5	C3—C2—C7	118.48 (17)	
O3—C8—H8B	109.5	C3—C2—C1	121.00 (16)	
H8A—C8—H8B	109.5	C7—C2—C1	120.51 (16)	
O3—C8—H8C	109.5	C2—C3—C4	121.22 (18)	
H8A—C8—H8C	109.5	C2—C3—H3	119.4	
H8B—C8—H8C	109.5	C4—C3—H3	119.4	
N3—C9—O3	119.7 (2)	C5—C4—C3	118.90 (18)	
N3—C9—C10	123.68 (19)	C5—C4—H4	120.5	
O3—C9—C10	116.64 (19)	C3—C4—H4	120.5	
C11—C10—C9	118.62 (18)	C6—C5—C4	121.40 (18)	
C11—C10—H10	120.7	C6—C5—Cl1	119.04 (16)	
C9—C10—H10	120.7	C4—C5—Cl1	119.55 (16)	
C10—C11—N1	117.9 (2)	C5—C6—C7	119.23 (18)	
C10—C11—C12	125.36 (19)	C5—C6—H6	120.4	
N1—C11—C12	116.74 (19)	C7—C6—H6	120.4	
C11—C12—H12A	109.5	C6—C7—C2	120.74 (18)	
C11—C12—H12B	109.5	C6—C7—H7	119.6	
H12A—C12—H12B	109.5	C2—C7—H7	119.6	
C11—C12—H12C	109.5			

O1—C1—C2—C3	−173.20 (19)	C4—C5—C6—C7	0.2 (3)
O1—C1—C2—C7	7.8 (3)	C5—C6—C7—C2	1.2 (3)
O2—C1—C2—C3	7.7 (3)	C13—N1—C11—C10	2.1 (3)
O2—C1—C2—C7	−171.35 (18)	C13—N1—C11—C12	−177.2 (2)
C1—C2—C3—C4	−177.99 (18)	C11—N1—C13—N2	179.63 (19)
C7—C2—C3—C4	1.0 (3)	C11—N1—C13—N3	−0.1 (3)
C1—C2—C7—C6	177.29 (19)	C13—N3—C9—O3	179.53 (18)
C3—C2—C7—C6	−1.8 (3)	C13—N3—C9—C10	−0.1 (3)
C2—C3—C4—C5	0.3 (3)	C9—N3—C13—N1	−0.9 (3)
C8—O3—C9—C10	176.7 (2)	C9—N3—C13—N2	179.37 (19)
C8—O3—C9—N3	−2.9 (3)	O3—C9—C10—C11	−177.6 (2)
C3—C4—C5—C6	−0.9 (3)	N3—C9—C10—C11	2.0 (4)
C3—C4—C5—Cl1	178.62 (16)	C9—C10—C11—N1	−2.9 (3)
Cl1—C5—C6—C7	−179.32 (16)	C9—C10—C11—C12	176.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O2	1.04 (3)	1.60 (3)	2.636 (3)	176 (2)
N2—H1*N*···O1[i]	0.86	2.12	2.846 (2)	142

N2—H2N···O1	0.86	1.97	2.824 (3)	169
C8—H8A···Cl1[ii]	0.96	2.82	3.770 (3)	171

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