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# 4-(Carboxymethyl)anilinium chloride

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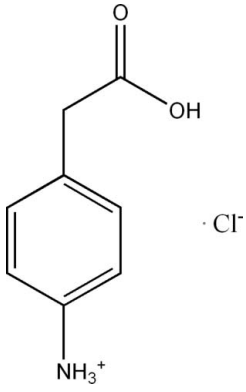
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.033; $wR$ factor = 0.080; data-to-parameter ratio = 17.8.

In the crystal of the title compound, $C_8H_{10}NO_2^+\cdot Cl^-$, alternating layers of hydrophobic and hydrophilic zones stack along the $c$ axis. The chloride anions are sandwiched between the 4-(carboxymethyl)anilinium layers, forming intermolecular O—H···Cl and N—H···Cl hydrogen bonds with the ammonium and carboxyl groups of the cations. In addition, intermolecular N—H···O and weak C—H···O and C—H···Cl hydrogen bonds help stabilize the crystal structure.

## Related literature

For our ongoing studies of hydrogen-bonding interactions in the crystal structures of protonated amines, see: Benslimane *et al.* (2007); Bouacida *et al.* (2005*a*,*b*,*c*, 2006, 2007, 2008, 2009). For amino acids in which the amino N atom is protonated, see: Bouacida *et al.* (2006); Rademeyer (2004*a*,*b*). For a related structure, see: Benslimane *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_8H_{10}NO_2^+\cdot Cl^-$
$M_r$ = 187.62
Monoclinic, $P2_1/n$
$a$ = 4.4982 (4) Å
$b$ = 11.0790 (11) Å
$c$ = 17.7120 (17) Å
$\beta$ = 95.429 (3)°
$V$ = 878.73 (14) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.39 mm$^{-1}$
$T$ = 100 K
0.44 × 0.12 × 0.1 mm

### Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min}$ = 0.809, $T_{max}$ = 0.962
7536 measured reflections
2006 independent reflections
1785 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.08
$S$ = 1.03
2006 reflections
113 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···Cl1$^{i}$ | 0.82 | 2.20 | 3.0087 (13) | 171 |
| N1—H1$A$···O2$^{ii}$ | 0.89 | 1.98 | 2.8517 (17) | 167 |
| N1—H1$B$···Cl1$^{iii}$ | 0.89 | 2.41 | 3.2285 (13) | 152 |
| N1—H1$C$···Cl1$^{iv}$ | 0.89 | 2.26 | 3.1516 (14) | 174 |
| C2—H2···O2$^{ii}$ | 0.93 | 2.49 | 3.2338 (18) | 137 |
| C3—H3···Cl1 | 0.93 | 2.82 | 3.7481 (15) | 175 |

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

Data collection: *APEX2* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2838).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Benslimane, M., Merazig, H., Bouacida, S., Denbri, S., Beghidja, A. & Ouahab, L. (2007). *Acta Cryst.* E**63**, o3682–o3683.
Bouacida, S. (2008). PhD thesis, Montouri–Constantine University, Algeria.
Bouacida, S., Belhouas, R., Kechout, H., Merazig, H. & Benard-Rocherulle, P. (2009). *Acta Cryst.* E**65**, o628–o629.
Bouacida, S., Merazig, H., Beghidja, A. & Beghidja, C. (2005*a*). *Acta Cryst.* E**61**, m1153–m1155.
Bouacida, S., Merazig, H., Beghidja, A. & Beghidja, C. (2005*b*). *Acta Cryst.* E**61**, m2072–m2074.

Bouacida, S., Merazig, H., Beghidja, A. & Beghidja, C. (2005*c*). *Acta Cryst.* E**61**, m577–m579.
Bouacida, S., Merazig, H. & Benard-Rocherulle, P. (2006). *Acta Cryst.* E**62**, o838–o840.
Bouacida, S., Merazig, H., Benard-Rocherulle, P. & Rizzoli, C. (2007). *Acta Cryst.* E**63**, m379–m381.
Brandenburg, K. & Berndt, M. (2001). *DIAMOND*. Version 3.1e. Crystal Impact, Bonn, Germany.
Bruker (1998). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Rademeyer, M. (2004*a*). *Acta Cryst.* C**60**, m55–m56.
Rademeyer, M. (2004*b*). *Acta Cryst.* E**60**, m345–m347.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2009). E**65**, o1563–o1564 [doi:10.1107/S1600536809021849]

## 4-(Carboxymethyl)anilinium chloride

**Habiba Kechout, Ratiba Belhouas, Sofiane Bouacida and Hocine Merazig**

### S1. Comment

The title compound, was prepared as part of our ongoing studies of hydrogen-bonding interactions in the crystal structure of protonated amines (Bouacida *et al.*, 2005*a*,*b*,*c*, 2006, 2007, 2008, 2009).

The molecular structure of (I), and the atomic numbering used, is illustrated in Fig. 1. All bond distances (Allen *et al.*, 1987) and angles are within the ranges of accepted values. The amino N atom is protonated as in previously reported amino acids (Bouacida & al., 2006; Rademeyer, 2004*a*,*b*). The layered crystal packing of (I) is shown in Fig. 2, in which cations form alterning layers of 4-(carboxymethyl)anilinium of hydrophobic and hydrophilic zones along the *c* axis, and the chloride ions are located between these layers. In the structure, two types of classical hydrogen bonds are observed, *viz*. cation–anion and cation–cation (Fig. 3). The 4-(carboxymethyl)anilinium cations and the chloride anions form hydrogen-bonded double layers at $z = 0$ and $z = 1/2$, linked by N—H···Cl, C—H···Cl and O—H···Cl hydrogen bonds. Additional hydrogen-bonding parameters are listed in Table 1. These interaction bonds link the cations and the anions together, forming a three-dimensional network and reinforcing the cohesion of the ionic structure.

### S2. Experimental

The title compound was crystallized by slow evaporation of an aqueous solution of 4-aminophenyl acetic acid, tin(II) chloride dihydrate and hydrochloric acid in a molar ratio of 5:5:1. White stick-like crystals were obtained after two weeks.

### S3. Refinement

All H atoms were located in Fourier maps but introduced in calculated positions and treated as riding on their parent C, O and N atoms with C—H = 0.93–0.97 Å, O—H = 0.82Å and N—H = 0.89Å and $U_{iso}$(H) =1.5–1.2(carrier atom).

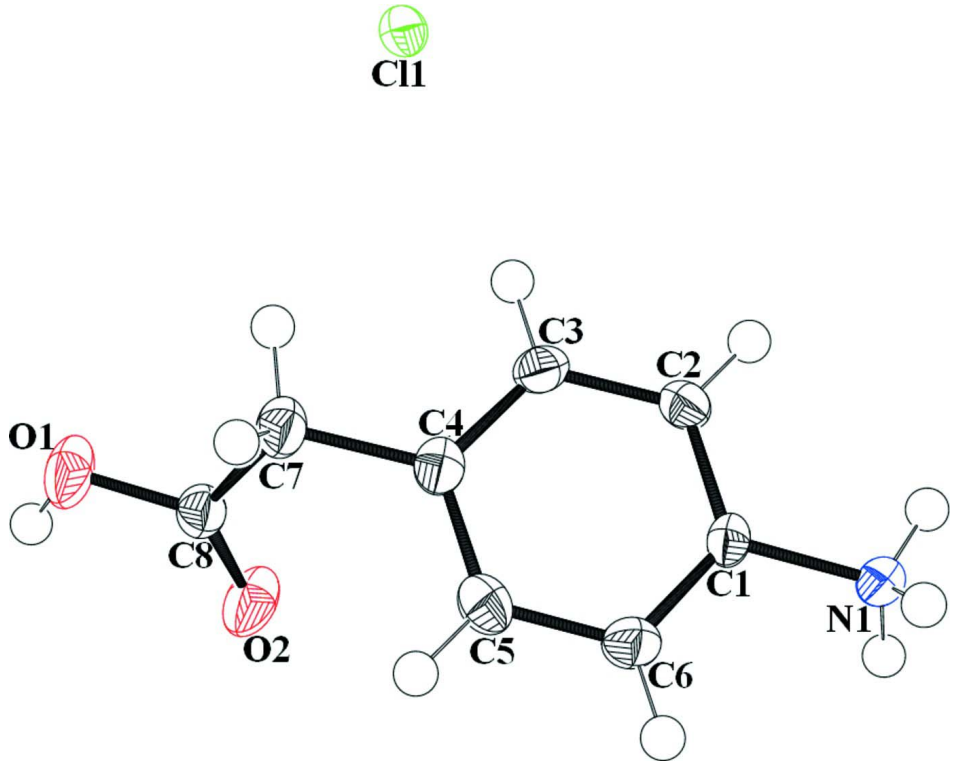


**Figure 1**

The asymmetric unit of the title compound with the atomic labelling scheme. Displacement are drawn at the 50% probability level.

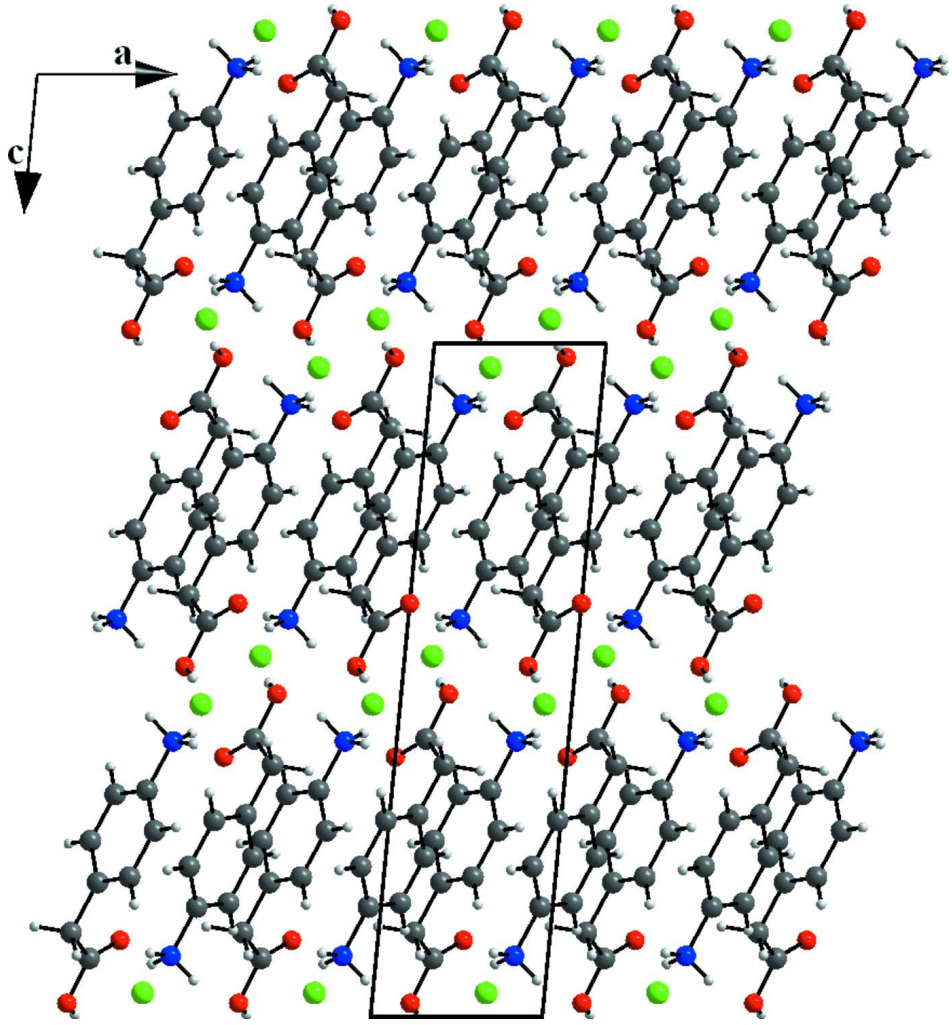


**Figure 2**

Part of the crystal structure illustrating the molecular layers, viewed along the *b* axis.

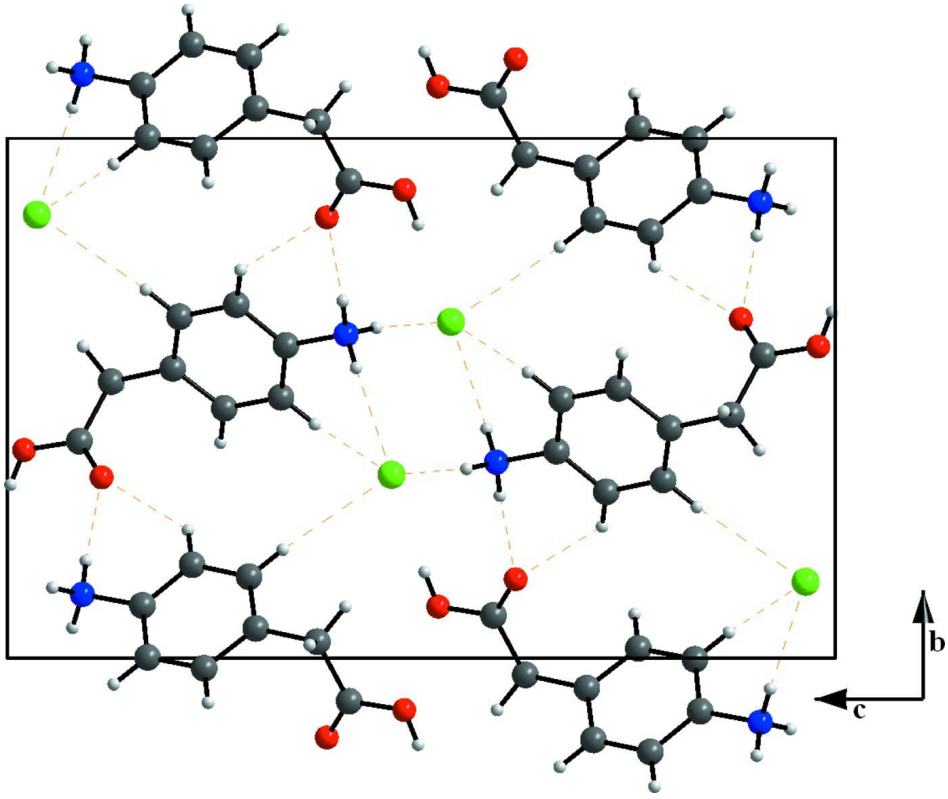


**Figure 3**

Part of the crystal structure with hydrogen bonds shown as dashed lines, viewed along the *a* axis.

### 4-(Carboxymethyl)anilinium chloride

*Crystal data*

$C_8H_{10}NO_2^+\cdot Cl^-$
$M_r = 187.62$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 4.4982\ (4)$ Å
$b = 11.0790\ (11)$ Å
$c = 17.7120\ (17)$ Å
$\beta = 95.429\ (3)°$
$V = 878.73\ (14)$ Å$^3$
$Z = 4$
$F(000) = 392$
$D_x = 1.418$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3208 reflections
$\theta = 2.3–27.4°$
$\mu = 0.39$ mm$^{-1}$
$T = 100$ K
Stick, white
0.44 × 0.12 × 0.1 mm

*Data collection*

Bruker APEXII diffractometer
Graphite monochromator
CCD rotation images, thin slices scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.809$, $T_{max} = 0.962$
7536 measured reflections
2006 independent reflections
1785 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.7°$
$h = -5\rightarrow5$
$k = -14\rightarrow14$
$l = -22\rightarrow22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.08$
$S = 1.03$
2006 reflections
113 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
$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 0.5301P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.22$ e Å$^{-3}$

*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.

**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 $F^2 > \sigma(F^2)$ 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 | 0.33999 (7) | 0.14718 (3) | 0.035821 (18) | 0.01567 (11) |
| O1 | 0.7756 (3) | 0.59938 (11) | 0.02054 (6) | 0.0270 (3) |
| H1 | 0.7238 | 0.6660 | 0.0040 | 0.040* |
| O2 | 0.5016 (3) | 0.65210 (10) | 0.11399 (6) | 0.0257 (3) |
| N1 | 0.3016 (3) | 0.37706 (11) | 0.40929 (7) | 0.0145 (3) |
| H1A | 0.1824 | 0.3128 | 0.4051 | 0.022* |
| H1B | 0.1969 | 0.4414 | 0.4212 | 0.022* |
| H1C | 0.4494 | 0.3642 | 0.4455 | 0.022* |
| C1 | 0.4271 (3) | 0.39836 (13) | 0.33671 (8) | 0.0126 (3) |
| C2 | 0.3601 (3) | 0.32006 (13) | 0.27659 (8) | 0.0148 (3) |
| H2 | 0.2377 | 0.2535 | 0.2817 | 0.018* |
| C3 | 0.4804 (3) | 0.34312 (13) | 0.20801 (8) | 0.0155 (3) |
| H3 | 0.4373 | 0.2911 | 0.1672 | 0.019* |
| C4 | 0.6631 (3) | 0.44257 (13) | 0.19984 (8) | 0.0145 (3) |
| C5 | 0.7279 (3) | 0.51913 (14) | 0.26215 (8) | 0.0176 (3) |
| H5 | 0.8524 | 0.5853 | 0.2576 | 0.021* |
| C6 | 0.6098 (3) | 0.49813 (14) | 0.33049 (8) | 0.0166 (3) |
| H6 | 0.6522 | 0.5499 | 0.3714 | 0.020* |
| C7 | 0.7903 (3) | 0.46817 (14) | 0.12557 (8) | 0.0180 (3) |
| H7A | 0.7456 | 0.4006 | 0.0916 | 0.022* |
| H7B | 1.0060 | 0.4744 | 0.1347 | 0.022* |
| C8 | 0.6709 (3) | 0.58249 (14) | 0.08711 (8) | 0.0157 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.01972 (19) | 0.01379 (19) | 0.01353 (18) | 0.00041 (13) | 0.00178 (13) | 0.00186 (12) |
| O1 | 0.0392 (7) | 0.0206 (6) | 0.0239 (6) | 0.0128 (5) | 0.0181 (5) | 0.0103 (5) |
| O2 | 0.0361 (7) | 0.0226 (6) | 0.0203 (6) | 0.0151 (5) | 0.0123 (5) | 0.0061 (5) |
| N1 | 0.0169 (6) | 0.0146 (6) | 0.0124 (6) | −0.0011 (5) | 0.0034 (5) | −0.0013 (5) |
| C4 | 0.0141 (6) | 0.0146 (7) | 0.0150 (7) | 0.0054 (5) | 0.0026 (5) | 0.0034 (5) |
| C1 | 0.0131 (6) | 0.0142 (7) | 0.0108 (6) | 0.0020 (5) | 0.0025 (5) | 0.0023 (5) |
| C6 | 0.0173 (7) | 0.0163 (7) | 0.0160 (7) | −0.0025 (6) | 0.0003 (5) | −0.0027 (6) |
| C3 | 0.0190 (7) | 0.0138 (7) | 0.0137 (7) | 0.0024 (6) | 0.0011 (5) | −0.0020 (5) |
| C7 | 0.0199 (7) | 0.0173 (7) | 0.0178 (7) | 0.0043 (6) | 0.0071 (6) | 0.0034 (6) |
| C8 | 0.0156 (7) | 0.0161 (7) | 0.0157 (7) | 0.0003 (6) | 0.0034 (5) | 0.0007 (6) |
| C5 | 0.0152 (7) | 0.0173 (7) | 0.0206 (7) | −0.0039 (6) | 0.0032 (5) | 0.0013 (6) |
| C2 | 0.0161 (6) | 0.0123 (7) | 0.0159 (7) | −0.0021 (6) | 0.0014 (5) | 0.0000 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C8 | 1.3234 (17) | C1—C6 | 1.388 (2) |
| O1—H1 | 0.8200 | C6—C5 | 1.387 (2) |
| O2—C8 | 1.2121 (18) | C6—H6 | 0.9300 |
| N1—C1 | 1.4709 (17) | C3—C2 | 1.399 (2) |
| N1—H1A | 0.8900 | C3—H3 | 0.9300 |
| N1—H1B | 0.8900 | C7—C8 | 1.512 (2) |
| N1—H1C | 0.8900 | C7—H7A | 0.9700 |
| C4—C3 | 1.390 (2) | C7—H7B | 0.9700 |
| C4—C5 | 1.401 (2) | C5—H5 | 0.9300 |
| C4—C7 | 1.5100 (19) | C2—H2 | 0.9300 |
| C1—C2 | 1.384 (2) | | |
| | | | |
| C8—O1—H1 | 109.5 | C4—C3—H3 | 119.5 |
| C1—N1—H1A | 109.5 | C2—C3—H3 | 119.5 |
| C1—N1—H1B | 109.5 | C4—C7—C8 | 113.72 (12) |
| H1A—N1—H1B | 109.5 | C4—C7—H7A | 108.8 |
| C1—N1—H1C | 109.5 | C8—C7—H7A | 108.8 |
| H1A—N1—H1C | 109.5 | C4—C7—H7B | 108.8 |
| H1B—N1—H1C | 109.5 | C8—C7—H7B | 108.8 |
| C3—C4—C5 | 118.62 (13) | H7A—C7—H7B | 107.7 |
| C3—C4—C7 | 121.06 (13) | O2—C8—O1 | 123.32 (14) |
| C5—C4—C7 | 120.33 (13) | O2—C8—C7 | 124.41 (13) |
| C2—C1—C6 | 121.69 (13) | O1—C8—C7 | 112.27 (12) |
| C2—C1—N1 | 119.89 (12) | C6—C5—C4 | 121.20 (14) |
| C6—C1—N1 | 118.42 (12) | C6—C5—H5 | 119.4 |
| C5—C6—C1 | 118.77 (13) | C4—C5—H5 | 119.4 |
| C5—C6—H6 | 120.6 | C1—C2—C3 | 118.67 (13) |
| C1—C6—H6 | 120.6 | C1—C2—H2 | 120.7 |
| C4—C3—C2 | 121.05 (13) | C3—C2—H2 | 120.7 |

| | | | |
|---|---|---|---|
| C2—C1—C6—C5 | −0.1 (2) | C4—C7—C8—O1 | −176.97 (13) |
| N1—C1—C6—C5 | −179.72 (13) | C1—C6—C5—C4 | 0.7 (2) |
| C5—C4—C3—C2 | 0.7 (2) | C3—C4—C5—C6 | −1.0 (2) |
| C7—C4—C3—C2 | −179.38 (13) | C7—C4—C5—C6 | 179.07 (13) |
| C3—C4—C7—C8 | 113.71 (16) | C6—C1—C2—C3 | −0.2 (2) |
| C5—C4—C7—C8 | −66.37 (18) | N1—C1—C2—C3 | 179.42 (12) |
| C4—C7—C8—O2 | 3.9 (2) | C4—C3—C2—C1 | −0.1 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···Cl1$^{i}$ | 0.82 | 2.20 | 3.0087 (13) | 171 |
| N1—H1*A*···O2$^{ii}$ | 0.89 | 1.98 | 2.8517 (17) | 167 |
| N1—H1*B*···Cl1$^{iii}$ | 0.89 | 2.41 | 3.2285 (13) | 152 |
| N1—H1*C*···Cl1$^{iv}$ | 0.89 | 2.26 | 3.1516 (14) | 174 |
| C2—H2···O2$^{ii}$ | 0.93 | 2.49 | 3.2338 (18) | 137 |
| C3—H3···Cl1 | 0.93 | 2.82 | 3.7481 (15) | 175 |

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