Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2-Carboxyanilinium chloride monohydrate

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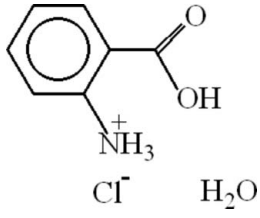
Received 6 September 2008; accepted 12 September 2008

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.102; data-to-parameter ratio = 16.1.

In the molecule of the title compound, $C_7H_8NO_2^+\cdot Cl^-\cdot H_2O$, an intramolecular N—H···O hydrogen bond results in the formation of a non-planar six-membered ring adopting a flattened boat conformation. In the crystal structure, intermolecular O—H···O and N—H···Cl hydrogen bonds link the molecules. There is a C=O···$\pi$ contact between the carbonyl unit and the centroid of the benzene ring. There is a C=O···$\pi$ contact [C···$Cg$ = 3.5802 (18), C—O···$Cg$ = 89 (1)°] between the carbonyl unit and the centroid of the benzene ring.

## Related literature

For applications of anthranilic acid derivatives, see: Congiu *et al.* (2005); Nittoli *et al.* (2005). For a related structure, see: Bahadur *et al.* (2007); For bond-length data, see: Allen *et al.* (1987). For ring puckering parameters, see: Cremer & Pople (1975).




## Experimental

### Crystal data

$C_7H_8NO_2^+\cdot Cl^-\cdot H_2O$
$M_r$ = 191.61
Monoclinic, $C2/c$
$a$ = 23.094 (4) Å
$b$ = 4.7833 (8) Å
$c$ = 16.381 (3) Å
$\beta$ = 91.605 (9)°
$V$ = 1808.8 (5) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.39 mm$^{-1}$
$T$ = 296 (2) K
0.28 × 0.10 × 0.06 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.975, $T_{max}$ = 0.985
9747 measured reflections
2238 independent reflections
1749 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
$S$ = 1.05
2238 reflections
139 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 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···O3$^{i}$ | 0.82 (2) | 1.73 (2) | 2.539 (2) | 171 (2) |
| N1—H1$A$···O2 | 0.91 (2) | 1.91 (2) | 2.6820 (19) | 142.1 (18) |
| N1—H1$B$···Cl1$^{ii}$ | 0.88 (2) | 2.28 (2) | 3.1464 (16) | 166.6 (18) |
| N1—H1$C$···Cl1$^{iii}$ | 0.958 (19) | 2.181 (19) | 3.1231 (16) | 167.5 (18) |
| O3—H3$A$···Cl1 | 0.76 (3) | 2.42 (3) | 3.1452 (18) | 160 (3) |
| O3—H3$B$···O2$^{iv}$ | 0.78 (3) | 2.04 (3) | 2.777 (3) | 159 (3) |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999) and *PLATON*.

The authors acknowledge the Higher Education Commission, Islamabad, Pakistan, for funding the purchase of the diffractometer at GCU, Lahore.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2527).

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# supporting information

*Acta Cryst.* (2008). E**64**, o1957 [doi:10.1107/S1600536808029267]

## 2-Carboxyanilinium chloride monohydrate

**Syed Azeem Rashid Ali Zaidi, M. Nawaz Tahir, Javed Iqbal and Muhammad Ashraf Chaudhary**

### S1. Comment

Anthranilic acid is widely used for various purposes such as production of dyes, pigments and saccharin. Its derivatives also have importance in medicinal chemistry and are used as antiinflammatory and anticancer agents (Congiu *et al.*, 2005) and for inhibition of Hepatitis C NS5B polymerase (Nittoli *et al.*, 2005). The title compound has been prepared to see its bioactivity with hope that it will be a good antibactarial agent at the economical cost and to utilize for preparing further derivatives. Crystal structures of proton transfer compound of 2-aminobenzoic acid with nitric acid (Bahadur *et al.*, 2007) has been reported, where the intramolecular N-H···O hydrogen bond has also been observed.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Ring A (C2-C7) is, of course, planar. The intramolecular N-H···O hydrogen bond (Table 1) results in the formation of a nonplanar six-membered ring B (N1/O2/C1/C2/C7/H1A) having total puckering amplitude, $Q_T$, of 0.127 (3) Å, and flattened boat conformation [$\varphi$ = -21.25 (3)°, $\theta$ = 44.41 (3)°] (Cremer & Pople, 1975).

In the crystal structure, intermolecular O-H···O and N-H···Cl hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure. The C=O···$\pi$ contact (Table 1) between the carbonyl moiety and the centroid of the benzene ring may further stabilize the structure.

### S2. Experimental

For the preparation of the title compound, 2-aminobenzoic acid (4.11 g, 3 mmol) and trichloroacetic acid (1.64 g, 1 mmol) were neutrilized with $Na_2CO_3$ separately in $H_2O$, and then mixed together. $Na_2CO_3$ (3.18 g) was added to the resulting mixture and refluxed for 4 h. The refluxed solution was cooled, and concenterated HCl was added to get PH = 1. The solution was kept in open air for 3 d to get the suitable crystals.

### S3. Refinement

H atoms were located in difference syntheses and refined as [O-H = 0.82 (2) Å (for OH); O-H = 0.76 (3) and 0.78 (3) Å (for $H_2O$); N-H = 0.88 (2)-0.958 (19) Å, ( for $NH_3$) and C-H = 0.93 (2)-0.96 (2) Å (for CH)] and constrained to ride on their parent atoms with $U_{iso}(H) = xU_{eq}(C,N,O)$, where x = 1.5 for $NH_3$ H and x = 1.2 for all other H atoms.

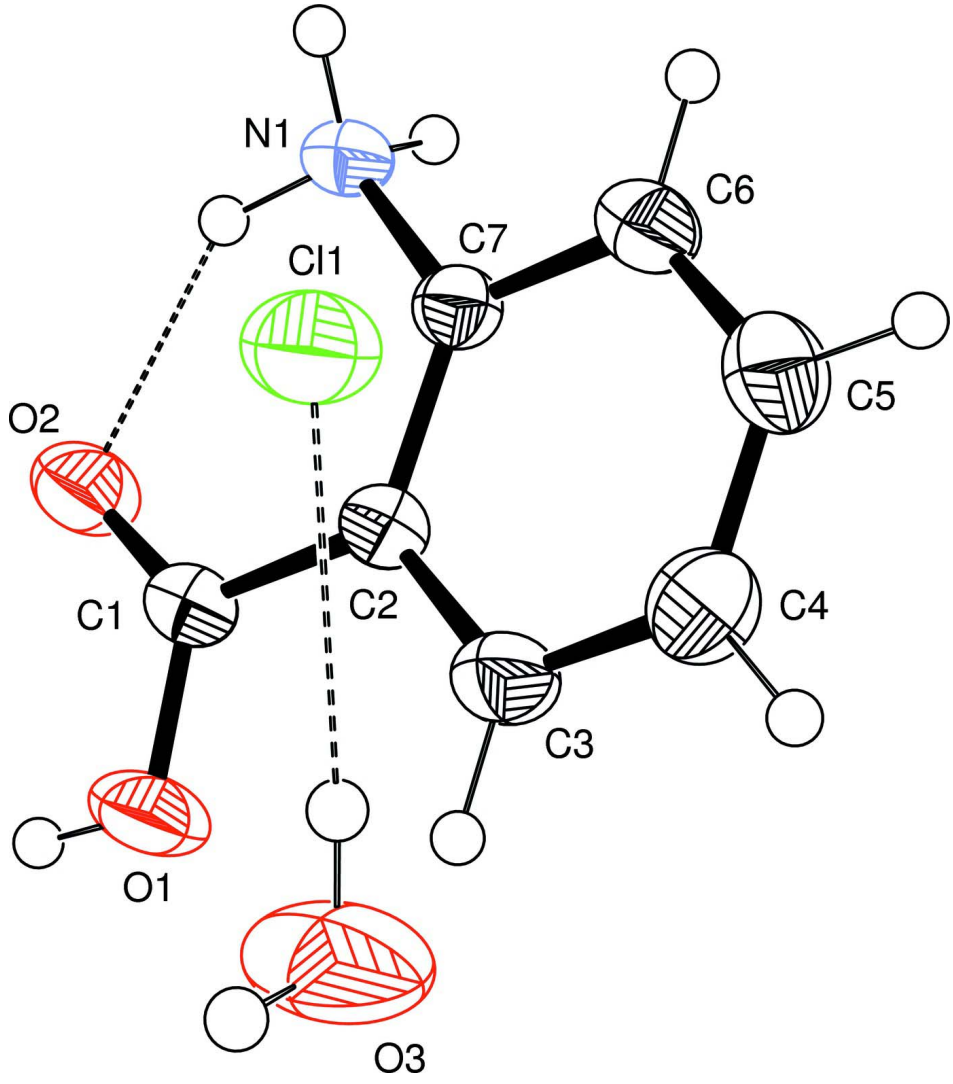


**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

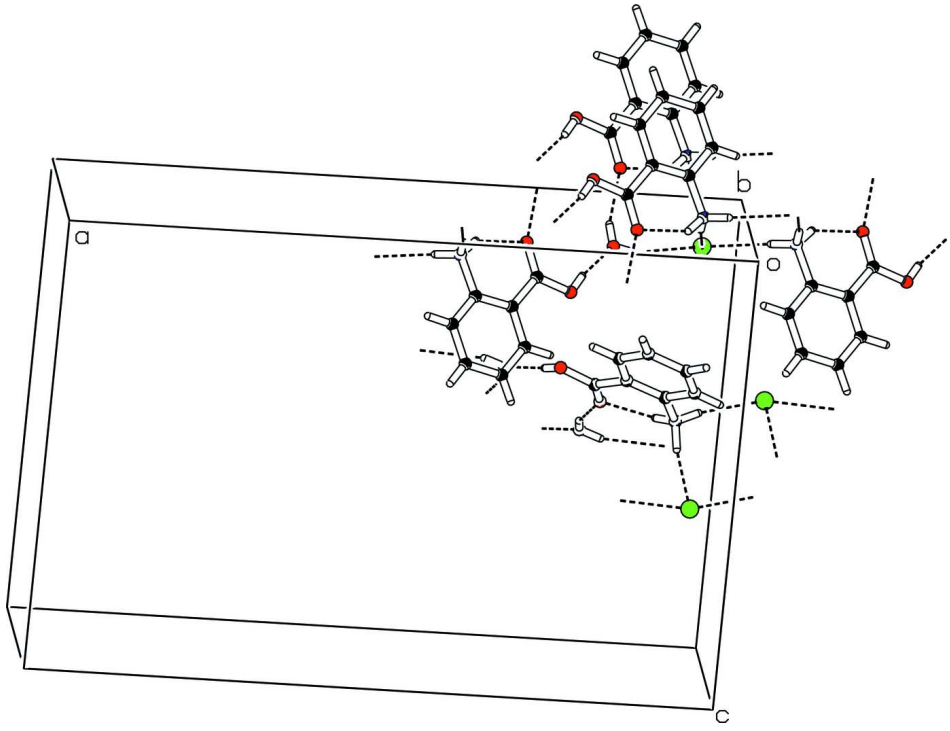


**Figure 2**

A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

### 2-Carboxyanilinium chloride monohydrate

*Crystal data*

$C_7H_8NO_2^+\cdot Cl^-\cdot H_2O$
$M_r = 191.61$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 23.094\ (4)$ Å
$b = 4.7833\ (8)$ Å
$c = 16.381\ (3)$ Å
$\beta = 91.605\ (9)°$
$V = 1808.8\ (5)$ Å$^3$
$Z = 8$
$F(000) = 800$
$D_x = 1.407$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2238 reflections
$\theta = 2.5–28.3°$
$\mu = 0.39$ mm$^{-1}$
$T = 296$ K
Prism, brown
0.28 × 0.10 × 0.06 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.5 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.975$, $T_{max} = 0.985$
9747 measured reflections
2238 independent reflections
1749 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.5°$
$h = -30\rightarrow30$
$k = -6\rightarrow3$
$l = -21\rightarrow20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.101$
$S = 1.05$
2238 reflections
139 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 1.0872P]$ 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**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 | 0.05634 (2) | 0.81018 (10) | 0.08328 (3) | 0.0425 (2) |
| O1 | 0.24332 (5) | 0.7928 (3) | 0.36801 (9) | 0.0551 (5) |
| O2 | 0.17708 (5) | 0.9236 (3) | 0.45555 (8) | 0.0493 (4) |
| O3 | 0.18909 (7) | 0.6690 (4) | 0.07558 (14) | 0.0796 (7) |
| N1 | 0.07438 (6) | 0.6617 (3) | 0.45470 (9) | 0.0340 (4) |
| C1 | 0.19199 (7) | 0.7781 (3) | 0.39900 (10) | 0.0338 (5) |
| C2 | 0.15328 (6) | 0.5699 (3) | 0.35784 (9) | 0.0304 (4) |
| C3 | 0.17259 (8) | 0.4219 (4) | 0.29012 (10) | 0.0408 (5) |
| C4 | 0.13710 (9) | 0.2318 (4) | 0.25017 (11) | 0.0462 (6) |
| C5 | 0.08157 (8) | 0.1841 (4) | 0.27706 (12) | 0.0466 (6) |
| C6 | 0.06160 (7) | 0.3269 (4) | 0.34388 (11) | 0.0398 (5) |
| C7 | 0.09727 (6) | 0.5188 (3) | 0.38354 (9) | 0.0300 (4) |
| H1 | 0.2619 (10) | 0.922 (5) | 0.3885 (14) | 0.0661* |
| H1A | 0.0991 (9) | 0.802 (4) | 0.4684 (12) | 0.0510* |
| H1B | 0.0399 (10) | 0.732 (4) | 0.4423 (13) | 0.0510* |
| H1C | 0.0724 (9) | 0.534 (4) | 0.4996 (12) | 0.0510* |
| H3 | 0.2113 (9) | 0.452 (4) | 0.2717 (11) | 0.0489* |
| H3A | 0.1584 (14) | 0.692 (7) | 0.0892 (19) | 0.0955* |
| H3B | 0.1945 (14) | 0.777 (6) | 0.041 (2) | 0.0955* |
| H4 | 0.1511 (9) | 0.133 (5) | 0.2061 (13) | 0.0554* |
| H5 | 0.0582 (9) | 0.052 (4) | 0.2493 (12) | 0.0558* |
| H6 | 0.0245 (9) | 0.298 (4) | 0.3628 (12) | 0.0477* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0314 (2) | 0.0499 (3) | 0.0463 (3) | −0.0004 (2) | 0.0035 (2) | −0.0055 (2) |
| O1 | 0.0320 (7) | 0.0668 (9) | 0.0673 (9) | −0.0189 (6) | 0.0174 (6) | −0.0255 (7) |
| O2 | 0.0401 (7) | 0.0554 (8) | 0.0531 (7) | −0.0144 (6) | 0.0133 (6) | −0.0206 (6) |
| O3 | 0.0408 (8) | 0.0837 (13) | 0.1153 (15) | 0.0249 (8) | 0.0207 (9) | 0.0514 (11) |
| N1 | 0.0255 (7) | 0.0362 (8) | 0.0406 (8) | −0.0012 (6) | 0.0081 (5) | −0.0030 (6) |
| C1 | 0.0283 (8) | 0.0362 (8) | 0.0372 (8) | −0.0030 (6) | 0.0049 (6) | 0.0006 (7) |
| C2 | 0.0279 (7) | 0.0312 (8) | 0.0323 (7) | −0.0017 (6) | 0.0041 (6) | 0.0009 (6) |
| C3 | 0.0357 (9) | 0.0456 (10) | 0.0416 (9) | −0.0040 (8) | 0.0111 (7) | −0.0063 (8) |
| C4 | 0.0512 (11) | 0.0487 (10) | 0.0391 (9) | −0.0031 (8) | 0.0077 (8) | −0.0135 (8) |
| C5 | 0.0445 (10) | 0.0462 (10) | 0.0486 (10) | −0.0088 (8) | −0.0048 (8) | −0.0109 (8) |
| C6 | 0.0292 (8) | 0.0435 (10) | 0.0466 (9) | −0.0053 (7) | 0.0018 (7) | −0.0030 (8) |
| C7 | 0.0278 (7) | 0.0307 (8) | 0.0315 (7) | 0.0005 (6) | 0.0031 (6) | 0.0014 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.304 (2) | C2—C3 | 1.399 (2) |
| O2—C1 | 1.216 (2) | C2—C7 | 1.393 (2) |
| O1—H1 | 0.82 (2) | C3—C4 | 1.377 (3) |
| O3—H3B | 0.78 (3) | C4—C5 | 1.387 (3) |
| O3—H3A | 0.76 (3) | C5—C6 | 1.380 (3) |
| N1—C7 | 1.463 (2) | C6—C7 | 1.383 (2) |
| N1—H1B | 0.88 (2) | C3—H3 | 0.96 (2) |
| N1—H1C | 0.958 (19) | C4—H4 | 0.93 (2) |
| N1—H1A | 0.91 (2) | C5—H5 | 0.94 (2) |
| C1—C2 | 1.487 (2) | C6—H6 | 0.93 (2) |
| | | | |
| Cl1···O3 | 3.1452 (18) | N1···O2 | 2.6820 (19) |
| Cl1···N1$^{i}$ | 3.3227 (16) | C1···C3$^{iv}$ | 3.581 (2) |
| Cl1···N1$^{ii}$ | 3.1464 (16) | C1···O3$^{vi}$ | 3.339 (2) |
| Cl1···N1$^{iii}$ | 3.1231 (16) | C1···C4$^{iv}$ | 3.477 (3) |
| Cl1···H5$^{iv}$ | 2.96 (2) | C3···C1$^{x}$ | 3.581 (2) |
| Cl1···H3A | 2.42 (3) | C3···O1$^{viii}$ | 3.338 (2) |
| Cl1···H6$^{v}$ | 3.13 (2) | C4···C1$^{x}$ | 3.477 (3) |
| Cl1···H1B$^{ii}$ | 2.28 (2) | C1···H1A | 2.46 (2) |
| Cl1···H1A$^{i}$ | 2.84 (2) | H1···H3B$^{vi}$ | 2.27 (4) |
| Cl1···H1C$^{iii}$ | 2.181 (19) | H1···H3A$^{vi}$ | 2.27 (4) |
| O1···C3$^{vi}$ | 3.338 (2) | H1···O3$^{vi}$ | 1.73 (2) |
| O1···O3$^{vi}$ | 2.539 (2) | H1A···C1 | 2.46 (2) |
| O2···O3$^{vii}$ | 2.777 (3) | H1A···O2 | 1.91 (2) |
| O2···N1 | 2.6820 (19) | H1A···Cl1$^{vii}$ | 2.84 (2) |
| O3···O2$^{i}$ | 2.777 (3) | H1B···Cl1$^{ii}$ | 2.28 (2) |
| O3···O1$^{viii}$ | 2.539 (2) | H1B···H6 | 2.47 (3) |
| O3···C1$^{viii}$ | 3.339 (2) | H1C···Cl1$^{ix}$ | 2.181 (19) |
| O3···Cl1 | 3.1452 (18) | H3···O1 | 2.372 (19) |
| O1···H4$^{vi}$ | 2.86 (2) | H3···O1$^{viii}$ | 2.655 (19) |

| | | | |
|---|---|---|---|
| O1···H3$^{vi}$ | 2.655 (19) | H3A···O2$^{i}$ | 2.90 (3) |
| O1···H3 | 2.372 (19) | H3A···H1$^{viii}$ | 2.27 (4) |
| O2···H3A$^{vii}$ | 2.90 (3) | H3A···Cl1 | 2.42 (3) |
| O2···H3B$^{vii}$ | 2.04 (3) | H3B···H1$^{viii}$ | 2.27 (4) |
| O2···H1A | 1.91 (2) | H3B···O2$^{i}$ | 2.04 (3) |
| O3···H1$^{viii}$ | 1.73 (2) | H4···O1$^{viii}$ | 2.86 (2) |
| N1···Cl1$^{ix}$ | 3.1231 (16) | H5···Cl1$^{x}$ | 2.96 (2) |
| N1···Cl1$^{vii}$ | 3.3227 (16) | H6···Cl1$^{xi}$ | 3.13 (2) |
| N1···Cl1$^{ii}$ | 3.1464 (16) | H6···H1B | 2.47 (3) |
| | | | |
| C1—O1—H1 | 110.7 (16) | C3—C4—C5 | 120.07 (17) |
| H3A—O3—H3B | 107 (3) | C4—C5—C6 | 120.20 (17) |
| C7—N1—H1C | 109.9 (12) | C5—C6—C7 | 119.54 (15) |
| H1A—N1—H1B | 109.5 (18) | N1—C7—C2 | 121.21 (13) |
| H1B—N1—H1C | 110.9 (19) | C2—C7—C6 | 121.35 (14) |
| C7—N1—H1A | 107.7 (13) | N1—C7—C6 | 117.43 (13) |
| H1A—N1—H1C | 109.0 (17) | C2—C3—H3 | 119.5 (11) |
| C7—N1—H1B | 109.8 (14) | C4—C3—H3 | 119.7 (11) |
| O1—C1—O2 | 123.05 (15) | C5—C4—H4 | 120.6 (13) |
| O1—C1—C2 | 113.64 (14) | C3—C4—H4 | 119.3 (13) |
| O2—C1—C2 | 123.31 (15) | C4—C5—H5 | 118.7 (13) |
| C3—C2—C7 | 118.04 (14) | C6—C5—H5 | 121.1 (13) |
| C1—C2—C7 | 122.14 (13) | C5—C6—H6 | 121.5 (12) |
| C1—C2—C3 | 119.82 (14) | C7—C6—H6 | 119.0 (12) |
| C2—C3—C4 | 120.80 (17) | | |
| | | | |
| O1—C1—C2—C3 | −2.8 (2) | C3—C2—C7—N1 | 178.91 (14) |
| O1—C1—C2—C7 | 178.32 (14) | C3—C2—C7—C6 | 0.3 (2) |
| O2—C1—C2—C3 | 176.32 (16) | C2—C3—C4—C5 | −0.3 (3) |
| O2—C1—C2—C7 | −2.5 (2) | C3—C4—C5—C6 | 0.1 (3) |
| C1—C2—C3—C4 | −178.82 (16) | C4—C5—C6—C7 | 0.3 (3) |
| C7—C2—C3—C4 | 0.1 (2) | C5—C6—C7—N1 | −179.16 (16) |
| C1—C2—C7—N1 | −2.2 (2) | C5—C6—C7—C2 | −0.5 (3) |
| C1—C2—C7—C6 | 179.17 (15) | | |

Symmetry codes: (i) $x$, $-y+2$, $z-1/2$; (ii) $-x$, $y$, $-z+1/2$; (iii) $x$, $-y+1$, $z-1/2$; (iv) $x$, $y+1$, $z$; (v) $-x$, $y+1$, $-z+1/2$; (vi) $-x+1/2$, $y+1/2$, $-z+1/2$; (vii) $x$, $-y+2$, $z+1/2$; (viii) $-x+1/2$, $y-1/2$, $-z+1/2$; (ix) $x$, $-y+1$, $z+1/2$; (x) $x$, $y-1$, $z$; (xi) $-x$, $y-1$, $-z+1/2$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O3$^{vi}$ | 0.82 (2) | 1.73 (2) | 2.539 (2) | 171 (2) |
| N1—H1*A*···O2 | 0.91 (2) | 1.91 (2) | 2.6820 (19) | 142.1 (18) |
| N1—H1*B*···Cl1$^{ii}$ | 0.88 (2) | 2.28 (2) | 3.1464 (16) | 166.6 (18) |
| N1—H1*C*···Cl1$^{ix}$ | 0.958 (19) | 2.181 (19) | 3.1231 (16) | 167.5 (18) |
| O3—H3*A*···Cl1 | 0.76 (3) | 2.42 (3) | 3.1452 (18) | 160 (3) |

| | | | | |
|---|---|---|---|---|
| O3—H3*B*···O2$^{i}$ | 0.78 (3) | 2.04 (3) | 2.777 (3) | 159 (3) |
| C1—O2···*Cg*$^{iv}$ | 1.22 (1) | 3.40 (1) | 3.5802 (18) | 89 (1) |

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