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# 4-(2,3-Dimethylphenyl)piperazin-1-ium chloride monohydrate

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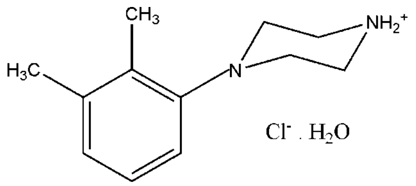
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.036; data-to-parameter ratio = 17.2.

The title compound, $C_{12}H_{19}N_2^+\cdot Cl^-\cdot H_2O$, contains a network of 4-(2,3-dimethylphenyl)piperazin-1-ium cations, water molecules and chloride anions. The crystal packing is influenced by O—H···Cl, N—H···Cl, N—H···O, C—H···O and C—H···Cl hydrogen bonds, resulting in structure with an open-framework architecture.

## Related literature

For related literature, see: Ben Gharbia *et al.* (2005, 2007); Bernstein *et al.* (1995); Pajewski *et al.* (2004); Sessler *et al.* (2003); Schmidtchen & Berge (1997). For the refinement weighting scheme, see: Prince (1982); Watkin (1994).



## Experimental

### Crystal data

$C_{12}H_{19}N_2^+\cdot Cl^-\cdot H_2O$
$M_r$ = 244.76
Triclinic, $P\bar{1}$
$a$ = 7.5439 (3) Å
$b$ = 9.4204 (3) Å
$c$ = 10.4347 (4) Å
$\alpha$ = 72.733 (2)°
$\beta$ = 74.152 (2)°
$\gamma$ = 70.250 (2)°
$V$ = 654.05 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 150 K
0.13 × 0.12 × 0.09 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
5719 measured reflections
3073 independent reflections
2601 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.035
$S$ = 1.10
2491 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H3···Cl1 | 0.90 | 2.18 | 3.069 (1) | 169 |
| N2—H4···O1$^{i}$ | 0.91 | 1.86 | 2.776 (2) | 175 |
| O1—H1···Cl1 | 0.82 | 2.32 | 3.120 (1) | 165 |
| O1—H2···Cl1$^{ii}$ | 0.83 | 2.31 | 3.136 (1) | 171 |
| C10—H15···Cl1$^{iii}$ | 0.99 | 2.87 | 3.846 (1) | 168 |
| C12—H20···Cl1$^{iv}$ | 0.97 | 2.84 | 3.779 (3) | 161 |
| C12—H19···O1$^{v}$ | 0.99 | 2.73 | 3.448 (2) | 130 |

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

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*/*SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *CRYSTALS*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2207).

## References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Ben Gharbia, I., Kefi, R., Rayes, A. & Ben Nasr, C. (2005). *Z. Kristallogr. New Cryst. Struct.*, **220**, 333–334.
Ben Gharbia, I., Kefi, R., Rayes, A. & Ben Nasr, C. (2007). *Anal. Sci. (X-Ray Str. Anal. Online)*, **27**, x243–x244.
Bernstein, J., David, R. E., Shimoni, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Nonius (2001). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Pajewski, R., Ferdani, R., Schlesinger, P.-H. & Gokel, G.-W. (2004). *Chem. Commun.* pp. 160–161.
Prince, E. (1982). *Mathematical Techniques in Crystallography and Materials Science*. New York: Springer.
Schmidtchen, F. P. & Berge, M. (1997). *Chem. Rev.* **97**, 1609–1646.
Sessler, J. L., Camiolo, S. & Gale, P. A. (2003). *Coord. Chem. Rev.* **240**, 17–150.
Watkin, D. (1994). *Acta Cryst.* A**50**, 411–437.

# supplementary materials

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# 4-(2,3-Dimethylphenyl)piperazin-1-ium chloride monohydrate

**I. Ben Gharbia, R. Kefi, M. El Glaoui, E. Jeanneau and C. Ben Nasr**

## Comment

The coordination chemistry of anions is a fast-growing area of supramolecular chemistry (Schmidtchen & Berge, 1997), on account of the importance of anion binding, recognition and transport in many biochemical processes (Pajewski *et al.*, 2004). Thus, the $Cl^-$ anion has been successfully used to assemble double-helical motifs of various molecules (Sessler *et al.*, 2003). Here a new member of this family, the title compound, is presented, which was obtained during our studies of the preparation of new organic hydrochloride compounds. As shown in Fig. 1, the asymmetric unit of the crystal structure of the title compound contains a 4-(2,3-dimethylphenyl)piperazin-1-ium cation, a chloride anion and a water molecule, associated in a hydrogen-bonded network. Two water molecules and two $Cl^-$ anions are interconnected through O—H···Cl hydrogen bonds, forming an 8-membered ring with graph-set $R_2^4(8)$ Bernstein *et al.*, 1995). These entities are connected to two antiparallel organic cations *via* N—H···Cl, N—H···O and C—H···Cl hydrogen-bonding interactions to construct a convoluted hydrogen-bonded chain which runs in the c-axis direction (Fig. 2). When projected along the *b* axis, the chains have a marked zigzag structure and somewhat resemble a helix (Fig. 3). In addition to the hydrogen-bonding associations to Cl1 and O1, the organic cations have a second role by linking these chains to each other to form layers parallel to the bc plane through C—H···O hydrogen bonds. Fig. 3 shows that these planes are interconnected by $NH_2^+$ groups to form an open framework architecture through hydrogen-bond interactions. An examination of the organic group geometrical features shows that the carbon atoms in the benzene ring of the title compound have a good coplanarity and they form a conjugated ring with an average deviation of 0.013 Å. The mean value of the C—C bond lengths [1.3967 (17) Å], which is between a single bond and a double bond, agrees with that in phenylpiperazinium tetrachloridozincate(II) [1.384 (4) Å] (Ben Gharbia *et al.*, 2005). The piperazine-1,4-diium ring of the title compound adopts a typical chair conformation and its geometric parameters [$d_{av}$(C—N) = 1.4818 (16) and $d_{av}$(C—C) = 1.5437 (17) Å] are in full agreement with those found in 4-(2,3-dimethylphenyl)piperazin-1-ium tetrachloridozincate(II) (Ben Gharbia *et al.*, 2007).

## Experimental

An aqueous 1*M* HCl solution and 1-(2,3-dimethylphenyl)piperazine in a 1:1 molar ratio were mixed and dissolved in sufficient ethanol. Crystals of (I) grew as the ethanol evaporated at 293 K over the course of a few days.

## Refinement

The H atoms were all located in a difference map, but those attached to carbon atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.98, N—H in the range 0.86–0.89 and O—H = 0.82 Å) and $U_{iso}$(H) (in the range 1.2–1.5 times $U_{eq}$ of the parent atom), after which the positions were refined with riding constraints. Low-angle reflections possibly affected by the beam-stop and some other outliers were omitted from the refinement.

## Figures

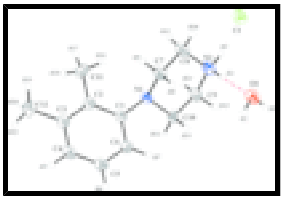

Fig. 1. The asymmetric unit of (I), showing 40% probability displacement ellipsoids.

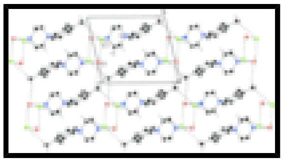

Fig. 2. The packing of (I), viewed down the *a* axis, showing the O—H···Cl, N—H···Cl, N—H···O, C—H···O and C—H···Cl interactions (dashed lines) between the 4-(2,3-dimethylphenyl)piperazin-1-ium cation, water molecule and chloride anion.

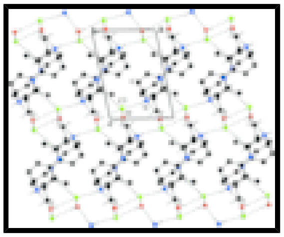

Fig. 3. The packing of (I), viewed down the *b* axis, showing the zigzag character of the structure. Hydrogen bonds are indicated by dashed lines.

### 4-(2,3-Dimethylphenyl)piperazin-1-ium chloride monohydrate

*Crystal data*

$C_{12}H_{19}N_2^+\cdot Cl^-\cdot H_2O$

$M_r = 244.76$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.5439\ (3)$ Å

$b = 9.4204\ (3)$ Å

$c = 10.4347\ (4)$ Å

$\alpha = 72.733\ (2)$°

$\beta = 74.152\ (2)$°

$\gamma = 70.250\ (2)$°

$V = 654.05\ (4)$ Å$^3$

$Z = 2$

$F_{000} = 264$

$D_x = 1.243$ Mg m$^{-3}$

Mo *K*α radiation
$\lambda = 0.71069$ Å

Cell parameters from 2750 reflections

$\theta = 0.4–27.9$°

$\mu = 0.28$ mm$^{-1}$

$T = 150$ K

Block, colorless

0.13 × 0.12 × 0.09 mm

*Data collection*

Nonius KappaCCD diffractometer

Monochromator: graphite

$T = 150$ K

φ and ω scans

Absorption correction: none

5719 measured reflections

3073 independent reflections

2601 reflections with $I > 2\sigma(I)$

$R_{int} = 0.016$

$\theta_{max} = 27.9$°

$\theta_{min} = 2.1$°

$h = -9\rightarrow9$

$k = -12\rightarrow12$

$l = -13\rightarrow13$

### *Refinement*

| | |
|---|---|
| Refinement on $F$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | $w = [1-(F_o-F_c)^2/36\sigma^2(F)]^2/[0.443T_0(x) + 0.129T_1(x) + 0.131T_2(x)]$<br>where $T_i$ are Chebychev polynomials and $x = F_c/F_{max}$ (Prince, 1982; Watkin, 1994) |
| $wR(F^2) = 0.035$ | $(\Delta/\sigma)_{max} = 0.0004$ |
| $S = 1.10$ | $\Delta\rho_{max} = 0.25$ e Å$^{-3}$ |
| 2491 reflections | $\Delta\rho_{min} = -0.20$ e Å$^{-3}$ |
| 145 parameters | Extinction correction: None |
| Primary atom site location: structure-invariant direct methods | |

### *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.09326 (17) | 0.26100 (14) | 0.53871 (13) | 0.0211 |
| C2 | −0.08069 (18) | 0.18226 (14) | 0.67481 (13) | 0.0224 |
| C3 | −0.24822 (19) | 0.15986 (14) | 0.76843 (13) | 0.0243 |
| C4 | −0.42381 (18) | 0.21709 (15) | 0.72522 (14) | 0.0270 |
| C5 | −0.43454 (18) | 0.29399 (16) | 0.59077 (14) | 0.0285 |
| C6 | −0.26999 (18) | 0.31526 (15) | 0.49687 (13) | 0.0255 |
| C7 | 0.18840 (18) | 0.14963 (15) | 0.38467 (14) | 0.0276 |
| C8 | 0.38588 (19) | 0.16564 (16) | 0.30991 (15) | 0.0313 |
| C9 | 0.24578 (19) | 0.45044 (15) | 0.26085 (13) | 0.0260 |
| C10 | 0.05184 (17) | 0.42554 (14) | 0.33543 (13) | 0.0230 |
| C11 | 0.1080 (2) | 0.12337 (17) | 0.72288 (15) | 0.0320 |
| C12 | −0.2398 (2) | 0.07656 (18) | 0.91485 (14) | 0.0353 |
| Cl1 | 0.77820 (5) | 0.34324 (4) | 0.11653 (4) | 0.0340 |
| O1 | 0.78625 (14) | 0.68790 (12) | 0.00994 (10) | 0.0353 |
| N1 | 0.07922 (14) | 0.28419 (12) | 0.44468 (11) | 0.0216 |
| N2 | 0.36750 (15) | 0.31276 (13) | 0.20308 (12) | 0.0278 |
| H1 | 0.7848 | 0.5995 | 0.0526 | 0.0528* |
| H2 | 0.9007 | 0.6873 | −0.0182 | 0.0528* |
| H3 | 0.4845 | 0.3270 | 0.1661 | 0.0430* |
| H4 | 0.3144 | 0.3085 | 0.1358 | 0.0437* |
| H5 | −0.5385 | 0.2058 | 0.7916 | 0.0322* |
| H6 | −0.5565 | 0.3352 | 0.5610 | 0.0341* |
| H7 | −0.2770 | 0.3659 | 0.4045 | 0.0295* |
| H8 | 0.1198 | 0.1410 | 0.3200 | 0.0321* |
| H9 | 0.2040 | 0.0561 | 0.4575 | 0.0315* |
| H10 | 0.4588 | 0.0790 | 0.2644 | 0.0369* |
| H11 | 0.4582 | 0.1695 | 0.3749 | 0.0356* |
| H12 | 0.3114 | 0.4642 | 0.3220 | 0.0314* |

| | | | | |
|---|---|---|---|---|
| H13 | 0.2299 | 0.5429 | 0.1850 | 0.0309* |
| H14 | −0.0266 | 0.5162 | 0.3773 | 0.0269* |
| H15 | −0.0141 | 0.4180 | 0.2684 | 0.0273* |
| H16 | 0.2087 | 0.1594 | 0.6514 | 0.0467* |
| H17 | 0.1484 | 0.0098 | 0.7464 | 0.0473* |
| H18 | 0.0940 | 0.1606 | 0.8047 | 0.0484* |
| H19 | −0.1476 | −0.0282 | 0.9197 | 0.0537* |
| H20 | −0.2011 | 0.1364 | 0.9587 | 0.0526* |
| H21 | −0.3671 | 0.0679 | 0.9639 | 0.0532* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0204 (5) | 0.0193 (5) | 0.0239 (6) | −0.0065 (4) | −0.0025 (4) | −0.0057 (5) |
| C2 | 0.0250 (6) | 0.0184 (5) | 0.0251 (6) | −0.0079 (5) | −0.0054 (5) | −0.0040 (5) |
| C3 | 0.0289 (6) | 0.0211 (6) | 0.0243 (6) | −0.0104 (5) | −0.0022 (5) | −0.0059 (5) |
| C4 | 0.0243 (6) | 0.0269 (6) | 0.0298 (7) | −0.0099 (5) | 0.0020 (5) | −0.0098 (5) |
| C5 | 0.0213 (6) | 0.0308 (7) | 0.0331 (7) | −0.0073 (5) | −0.0039 (5) | −0.0081 (6) |
| C6 | 0.0231 (6) | 0.0273 (6) | 0.0250 (6) | −0.0079 (5) | −0.0040 (5) | −0.0040 (5) |
| C7 | 0.0241 (6) | 0.0215 (6) | 0.0347 (7) | −0.0077 (5) | 0.0025 (5) | −0.0088 (5) |
| C8 | 0.0229 (6) | 0.0274 (7) | 0.0392 (8) | −0.0073 (5) | 0.0025 (5) | −0.0088 (6) |
| C9 | 0.0289 (6) | 0.0260 (6) | 0.0255 (6) | −0.0128 (5) | −0.0024 (5) | −0.0061 (5) |
| C10 | 0.0236 (6) | 0.0224 (6) | 0.0220 (6) | −0.0081 (5) | −0.0026 (5) | −0.0034 (5) |
| C11 | 0.0286 (7) | 0.0337 (7) | 0.0317 (7) | −0.0115 (6) | −0.0113 (5) | 0.0038 (6) |
| C12 | 0.0452 (8) | 0.0378 (8) | 0.0246 (7) | −0.0210 (7) | −0.0034 (6) | −0.0016 (6) |
| Cl1 | 0.02788 (17) | 0.0430 (2) | 0.03519 (18) | −0.01831 (14) | −0.00224 (13) | −0.00861 (14) |
| O1 | 0.0303 (5) | 0.0377 (6) | 0.0367 (5) | −0.0128 (4) | 0.0007 (4) | −0.0094 (4) |
| N1 | 0.0205 (5) | 0.0191 (5) | 0.0234 (5) | −0.0059 (4) | −0.0013 (4) | −0.0044 (4) |
| N2 | 0.0229 (5) | 0.0332 (6) | 0.0291 (6) | −0.0136 (4) | 0.0028 (4) | −0.0101 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C9—C10 | 1.5176 (17) | C6—H7 | 0.947 |
| C9—N2 | 1.4986 (17) | C5—C4 | 1.3851 (19) |
| C9—H12 | 0.966 | C5—H6 | 0.968 |
| C9—H13 | 0.985 | C4—C3 | 1.3957 (19) |
| C10—N1 | 1.4686 (16) | C4—H5 | 0.965 |
| C10—H14 | 1.005 | C3—C2 | 1.4070 (17) |
| C10—H15 | 0.993 | C3—C12 | 1.5038 (19) |
| C7—C8 | 1.5159 (17) | C2—C11 | 1.5090 (17) |
| C7—N1 | 1.4701 (16) | C12—H21 | 0.975 |
| C7—H9 | 0.974 | C12—H20 | 0.974 |
| C7—H8 | 0.991 | C12—H19 | 0.993 |
| C8—N2 | 1.4900 (18) | C11—H18 | 0.983 |
| C8—H11 | 0.995 | C11—H16 | 0.981 |
| C8—H10 | 0.989 | C11—H17 | 0.981 |
| C1—C6 | 1.3979 (17) | O1—H1 | 0.822 |
| C1—C2 | 1.4060 (17) | O1—H2 | 0.831 |
| C1—N1 | 1.4391 (15) | N2—H3 | 0.900 |

| | | | |
|---|---|---|---|
| C6—C5 | 1.3886 (18) | N2—H4 | 0.914 |
| C10—C9—N2 | 109.56 (10) | C4—C5—H6 | 120.8 |
| C10—C9—H12 | 111.0 | C5—C4—C3 | 120.72 (12) |
| N2—C9—H12 | 108.8 | C5—C4—H5 | 120.5 |
| C10—C9—H13 | 110.3 | C3—C4—H5 | 118.7 |
| N2—C9—H13 | 108.5 | C4—C3—C2 | 119.63 (12) |
| H12—C9—H13 | 108.6 | C4—C3—C12 | 119.84 (12) |
| C9—C10—N1 | 109.41 (10) | C2—C3—C12 | 120.53 (12) |
| C9—C10—H14 | 109.0 | C3—C2—C1 | 119.20 (11) |
| N1—C10—H14 | 108.9 | C3—C2—C11 | 119.40 (12) |
| C9—C10—H15 | 108.6 | C1—C2—C11 | 121.39 (11) |
| N1—C10—H15 | 111.3 | C3—C12—H21 | 109.5 |
| H14—C10—H15 | 109.6 | C3—C12—H20 | 109.5 |
| C8—C7—N1 | 110.04 (10) | H21—C12—H20 | 107.6 |
| C8—C7—H9 | 108.4 | C3—C12—H19 | 110.4 |
| N1—C7—H9 | 109.2 | H21—C12—H19 | 109.8 |
| C8—C7—H8 | 109.4 | H20—C12—H19 | 109.9 |
| N1—C7—H8 | 110.2 | C2—C11—H18 | 109.7 |
| H9—C7—H8 | 109.5 | C2—C11—H16 | 110.8 |
| C7—C8—N2 | 109.88 (11) | H18—C11—H16 | 109.0 |
| C7—C8—H11 | 110.1 | C2—C11—H17 | 110.4 |
| N2—C8—H11 | 107.8 | H18—C11—H17 | 108.5 |
| C7—C8—H10 | 111.2 | H16—C11—H17 | 108.4 |
| N2—C8—H10 | 108.0 | H1—O1—H2 | 107.1 |
| H11—C8—H10 | 109.9 | C7—N1—C10 | 109.62 (10) |
| C6—C1—C2 | 120.31 (11) | C7—N1—C1 | 112.16 (9) |
| C6—C1—N1 | 121.24 (11) | C10—N1—C1 | 115.19 (10) |
| C2—C1—N1 | 118.45 (11) | C9—N2—C8 | 112.04 (10) |
| C1—C6—C5 | 119.86 (12) | C9—N2—H3 | 107.5 |
| C1—C6—H7 | 119.9 | C8—N2—H3 | 109.3 |
| C5—C6—H7 | 120.2 | C9—N2—H4 | 108.6 |
| C6—C5—C4 | 120.27 (12) | C8—N2—H4 | 110.2 |
| C6—C5—H6 | 118.9 | H3—N2—H4 | 109.1 |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H3···Cl1 | 0.90 | 2.18 | 3.069 (1) | 169 |
| N2—H4···O1$^{i}$ | 0.91 | 1.86 | 2.776 (2) | 175 |
| O1—H1···Cl1 | 0.82 | 2.32 | 3.120 (1) | 165 |
| O1—H2···Cl1$^{ii}$ | 0.83 | 2.31 | 3.136 (1) | 171 |
| C10—H15···Cl1$^{iii}$ | 0.99 | 2.87 | 3.846 (1) | 168 |
| C12—H20···Cl1$^{iv}$ | 0.97 | 2.84 | 3.779 (3) | 161 |
| C12—H19···O1$^{v}$ | 0.99 | 2.73 | 3.448 (2) | 130 |

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

**Fig. 1**

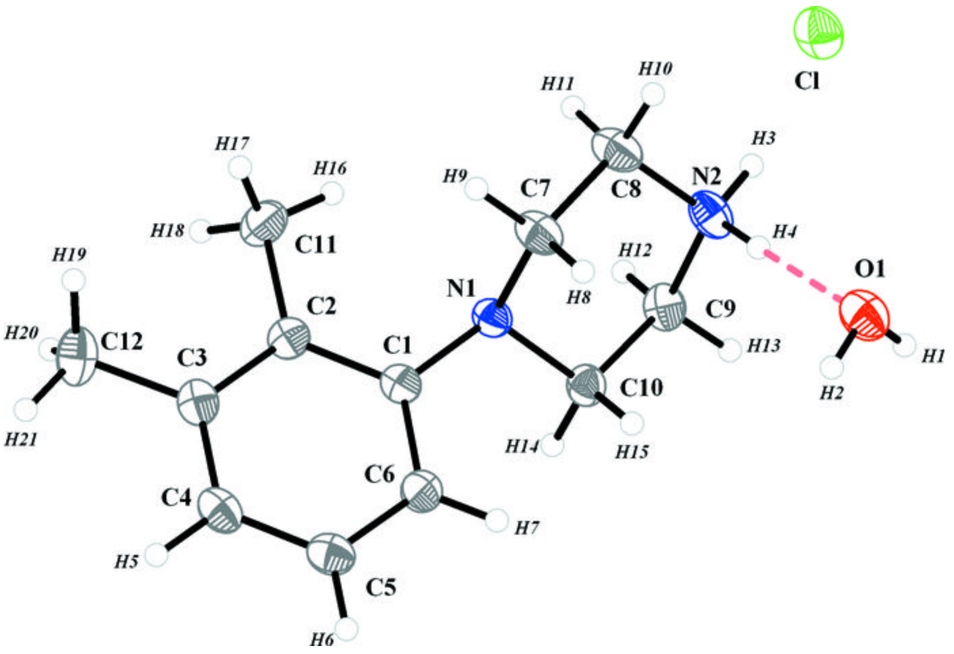
Cl
H11
H10
H3
H17
H16
H9
C7
C8
N2
H4
H18
C11
H12
O1
H19
N1
H8
C9
H20
C12
C3
C2
C1
H13
H1
C10
H2
H21
H14
H15
C6
C4
H7
H5
C5
H6

**Fig. 2**

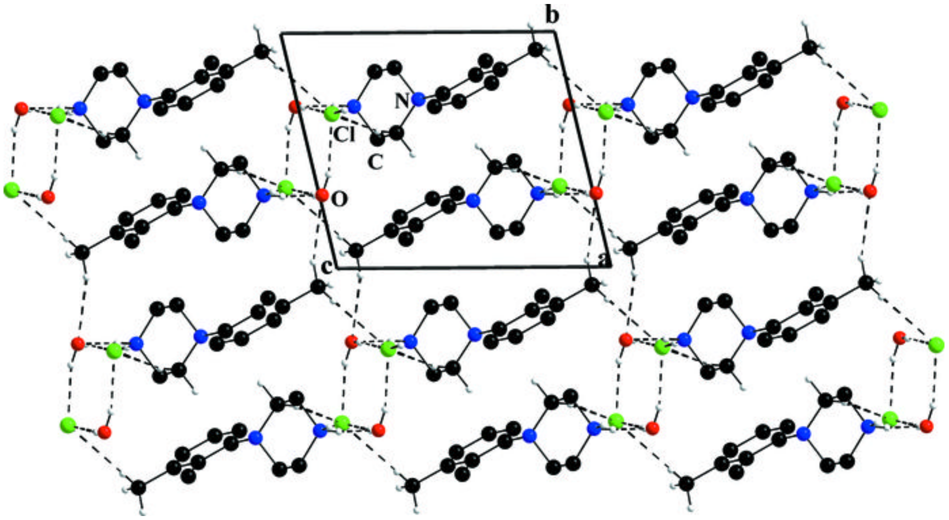

Fig. 3