Crystal structure of 1,1′-(pyridine-2,6-diyl)bis[N-(pyridin-2-ylmethyl)methanaminium] dichloride dihydrate

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In the title compound, C19H23N52+/C12Cl/C0/C12H2O, the two pyridine side arms are not coplanar, with the terminal pyridine rings subtending a dihedral angle of 26.45 (6)°. In the crystal, hydrogen bonds, intermolecular C—H ••• Cl contacts and a weak C—H ••• O interaction connect the molecule with neighbouring chloride counter-anions and lattice water molecules. The crystal packing also features by π–π interactions with centroid-centroid distances of 3.4864 (12) and 3.5129 (13) Å.

1. Chemical context

In recent years, ruthenium nitrosyl complexes have attracted considerable attention, essentially because of their interesting photoreactivity properties such as photochromism (Schaniel et al., 2007) and nitric oxide photorelease (Rose & Mascharak, 2008a). Ruthenium nitrosyl complexes could have desirable photoreactivity properties relying on the nature of the ligands. The utilization of polydentate ligands in coordination chemistry gives a few benefits over monodentate ligands, in particular because of the chelate effect (Martell, 1967). Multidentate pyridylamine derivative ligands can better control the stability (Afshar et al., 2004; Eroy-Reveles et al., 2007), solubility (Harrop et al., 2005) and structural characteristics of the resulting complex. More particularly, ruthenium complexes derived from pentadentate ligands are generally stable in physiological media (Halpenny et al., 2007; Rose & Mascharak, 2008b). This stability is necessary for (i) maintaining pharmacological activity, (ii) reducing the toxicity of free metal ions, and (iii) avoiding non-specific binding of partially connected metal ions with other biomolecules (Fry & Mascharak, 2011; Hoffman-Luca et al., 2009; Patra & Mascharak, 2003; Heilman et al., 2012). In the search for new systems, we report here the synthesis and crystal structure of 1,1′-(pyridine-2,6-diyl)bis[N-(pyridin-2-ylmethyl)methanaminium] dichloride dihydrate, which contains multiple coordination sites, and is thus an excellent candidate for forming stable ruthenium nitrosyl complexes.

2. Structural commentary

The title compound crystallizes in the triclinic space group P1 with one cationic molecule, two chloride anions, and two water
molecules per asymmetric unit. In the organic molecule, one terminal pyridine ring is almost co-planar with the central pyridine ring, making a dihedral angle of 4.56 (8)°, while the second terminal pyridine ring is out of the plane with a dihedral angle between the two terminal pyridine rings of 26.45 (6)° (Fig. 1). Bond lengths are within normal ranges and comparable with values found for a similar compound, \( \text{N,N'-dialkyl-2,6-pyridinedimethanaminium} \) (Kobayashi et al., 2006).

3. Supramolecular features

In the crystal, there are intermolecular hydrogen bonds (Table 1) and C—H···Cl and C—H···O interactions between the molecules, the chloride anions and the lattice water molecules. The molecular structure of the compound is illustrated in Fig. 1 with hydrogen bonding indicated.

![Figure 1](image1.png)

**Figure 1**
Molecular structure showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as small spheres of an arbitrary radius. The orange dashed lines represent hydrogen bonds, C—H···Cl interactions and the weak C—H···O interaction. [Symmetry codes: (i) \( x - 1, y, z \); (ii) \( x + 1, y, z \); (iii) \( x - 1, y + 1, z \); (iv) \(-x + 1, -y + 1, -z + 2 \); (v) \( x, y - 1, z \).]

![Figure 2](image2.png)

**Figure 2**
Views of the stacking along the \( a \) axis. Orange lines indicate \( \pi-\pi \) interactions. Displacement ellipsoids are drawn at the 50% probability level.

| \( D-H \cdots A \) | \( D-H \) | \( H \cdots A \) | \( D-A \) | \( D-H \cdots A \) |
|-------------------|--------|-------------|--------|-----------------|
| O2—H201···Cl1    | 0.85 (3) | 2.41 (3) | 3.1844 (15) | 152 (2)          |
| O2—H202···N5     | 0.91 (3) | 2.10 (3) | 2.947 (2) | 155 (2)          |
| N2—H21···O2      | 0.94 (2) | 1.89 (2) | 2.804 (2) | 165 (2)          |
| N2—H22···Cl1i    | 0.86 (2) | 2.31 (2) | 3.1446 (17) | 162.5 (17)       |
| N4—H41···Cl2     | 0.91 (2) | 2.25 (2) | 3.1319 (17) | 164.1 (19)       |
| N4—H42···O1i     | 0.97 (2) | 1.90 (2) | 2.825 (2) | 158 (2)          |
| O1—H101···Cl1    | 0.93 (3) | 2.43 (3) | 3.2611 (15) | 149 (2)          |
| O1—H102···N3ii   | 1.00 (4) | 1.93 (4) | 2.920 (2) | 172 (3)          |
| C3—H3···Cl1iii   | 0.95 | 2.73 | 3.5702 (19) | 148 |
| C6—H6A···Cl1     | 0.99 | 2.8 | 3.751 (2) | 161 |
| C7—H7A···Cl1ii   | 0.99 | 2.78 | 3.7351 (18) | 162 |
| C10—H10···Cl1i   | 0.95 | 2.71 | 3.6469 (18) | 168 |
| C17—H17···O1ii   | 0.95 | 2.57 | 3.437 (2) | 151 |

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

The crystal packing shows \( \pi-\pi \) interactions between two parallel neighbouring molecules along the \( a \)-axis direction with a \( \text{Cg}1 \cdot \cdot \cdot \text{Cg}2 \) (\( x, y - 1, z \)) centroid-centroid distance of 3.4864 (12) Å, a perpendicular distance from the centroid \( \text{Cg}1 \) to the plane of the other ring of 3.2472 (8) Å and a slippage between the centroids of 1.100 Å. Similarly, the second \( \pi-\pi \) stacking interaction has a \( \text{Cg}3 \cdot \cdot \cdot \text{Cg}3(\neg x, \neg y + 2, \neg z + 1) \) centroid-centroid distance of 3.5129 (13) Å, a perpendicular distance from the centroid \( \text{Cg}3 \) to the plane of the other ring of 3.2177 (8) Å and a slippage between the centroids of 1.410 Å. \( \text{Cg}1, \text{Cg}2 \) and \( \text{Cg}3 \) are the centroids of N1/C8–C12, N3/C1–C5 and N5/C15–C19 pyridine rings, respectively (Fig. 2).

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.42, last updated May 2021; Groom et al., 2016) for similar compounds gave three hits. They include \( \text{N,N'-bis(2-pyridylmethyl)pyridine-2,6-dicarboxamide} \) (CSD refcode AVURAK; Jain et al., 2004), \( \text{N,N'-bis[2-(2-pyridyl)methyl]pyridine-2,6-dicarboxamide hemihydrate} \) (HULKUU; Jian Ying Qi et al., 2006).
5. Synthesis and crystallization

1,1’-(Pyridine-2,6-diyl)bis[N-(pyridin-2-ylmethyl)ethanam-
inum] dichloride dihydrate compound was obtained following
the procedure previously reported in the literature (Gruen-
wedel, 1968; Newkome et al., 1984; Darbre et al., 2002;
Kobayashi et al., 2006). The procedure used for the synthesis
has three steps. Firstly, the synthesis of 2-[(tosylamino)meth-
yl]pyridine was carried out by treatment of 2-(aminomethyl)
pyridine with NaOH and tosyl chloride in a two-phase system
(water/diethyl ether) (Newkome et al., 1984). In the second
step, the coupling of 2-[(tosylamino)methyl]pyridine with 2,6-
bis(bromomethyl) pyridine, also in a two-phase system (di-
chloromethane/water) and nBu4NBr as phase-transfer catalyst
gave 2,6-bis[(pyridin-2-ylmethyl)tosyl]amino[methyl]pyridine,
which could be isolated after chromatography (Darbre et al.,
2002). Finally, the tosylate group of 2,6-bis[(pyridin-2-ylmeth-
yl)pyridine was removed using concentrated sulfuric acid for
deprotection with heating at 393 K for 3 h to give an unstable
brownish oil (Newkome et al., 1984).

Slow diffusion between toluene and a wet dichloromethane
solution of the brown oil set aside at room temperature gave
colourless needles of the title compound suitable for X-ray
diffraction within five days.

6. Refinement

Crystal data, data collection and structure refinement details
are summarized in Table 2. Hydrogen atoms of the water
molecules and those bonded to nitrogen atoms were located in
difference-Fourier maps and refined freely with isotropic
displacement parameters. All C-bound H atoms were placed
in calculated positions and refined using a riding model, with
C–H = 0.95 (aromatic) or 0.99 Å (methylene) and with
Uiso(H) = 1.2Ueq(C). For two similar N–H distances, a
restraint was applied to make them approximately equal with
an effective standard deviation of 0.02 Å.

| Crystal data | Chemical formula | C19H23N52+·2Cl−·2H2O |
|--------------|-----------------|------------------------|
| Acta Cryst. |                  |                        |
| B             |                 |                        |
| 0.35         |                 |                        |

Computer programs: APEX3 and SAINT (Bruker, 2012). SHELXT (Sheldrick 2015a),
SHELXL2018/3 (Sheldrick, 2015b), Mercury (Macrae et al., 2020) and pubCIF (Westrip,
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supporting information

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Crystal structure of 1,1′-(pyridine-2,6-diyl)bis[N-(pyridin-2-ylmethyl)methanaminium] dichloride dihydrate

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Computing details

Data collection: *APEX3* (Bruker, 2012); cell refinement: *APEX3* and *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXT* (Sheldrick 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *publCIF* (Westrip, 2010).

1,1′-(Pyridine-2,6-diyl)bis[N-(pyridin-2-ylmethyl)methanaminium] dichloride dihydrate

Crystal data

| Parameter               | Value                          |
|-------------------------|--------------------------------|
| formula                 | C_{19}H_{23}N_{5}·2Cl·2H_{2}O |
| Mr                      | 428.36                         |
| Space group             | Triclinic, *P*1                |
| Hall symbol             | -P1                            |
| *a*                     | 7.1579 (6) Å                   |
| *b*                     | 8.8119 (7) Å                   |
| *c*                     | 17.4150 (13) Å                 |
| *α*                     | 80.357 (3)°                    |
| *β*                     | 80.805 (3)°                    |
| *γ*                     | 68.919 (3)°                    |
| *V*                     | 1004.52 (14) Å                 |
| *Z*                     | 2                              |
| *F*(000)                | 452                            |
| *D*<sub>c</sub>         | 1.416 Mg m<sup>-3</sup>        |
| Radiation source        | Mo *Ka* radiation, *λ* = 0.71073 Å |
| Cell parameters         | *θ* = 3.2–31.4°                |
| Absorption correction   | *μ* = 0.35 mm<sup>−1</sup>     |
| Temperature             | *T* = 110 K                    |
| Needle, colourless      | *T* min = 0.660, *T* max = 0.746 |

Data collection

| Parameter               | Value                          |
|-------------------------|--------------------------------|
| Bruker Kappa APEXII Quazar diffractometer | 29584 measured reflections |
| Radiation source        | microfocus sealed tube         |
| Multilayer optics       | monochromator                   |
| phi and ω scans         |                                |
| Absorption correction   | multi-scan                      |
| (SADABS; Krause *et al.*, 2015) | 4632 reflections with *I* > 2σ(*I*) |
| *R*<sub>int</sub>       | 0.097                          |
| *θ* max, *θ* min        | 32.0°, 1.2°                    |
| *h*                     | -10→10                         |
| *k*                     | -13→13                         |
| *l*                     | -25→25                         |

Refinement

| Parameter               | Value                          |
|-------------------------|--------------------------------|
| Refinement on *F*<sup>2</sup> |                                 |
| Least-squares matrix    | full                           |
| *R*(*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)) | 0.05                           |
| *wR*(*F*<sup>2</sup>)    | 0.123                          |
| *S*                      | 1.03                           |
| 6970 reflections        |                                |
| 283 parameters          |                                |
| 1 restraint              |                                |

Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

*P* = (*F*<sup>2</sup> + 2*F*<sup>c</sup>)<sup>3</sup>/3
(Δ/σ)_{max} = 0.002
\Delta \rho_{max} = 0.45 \text{ e Å}^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|   | x      | y      | z      | Uiso*/Ueq |
|---|--------|--------|--------|-----------|
| C1| −0.0133 (3) | 1.1436 (2) | 0.77592 (11) | 0.0187 (4) |
| H1| −0.057178 | 1.157686 | 0.725689 | 0.022* |
| C2| −0.0514 (3) | 1.2816 (2) | 0.81173 (12) | 0.0209 (4) |
| H2| −0.118646 | 1.387618 | 0.786614 | 0.025* |
| C3| 0.0110 (3) | 1.2617 (2) | 0.88529 (12) | 0.0209 (4) |
| H3| −0.013857 | 1.353959 | 0.91186 | 0.025* |
| C4| 0.1098 (3) | 1.1057 (2) | 0.91921 (11) | 0.0177 (4) |
| H4| 0.15363 | 1.089007 | 0.969628 | 0.021* |
| C5| 0.1446 (3) | 0.9729 (2) | 0.87872 (10) | 0.0141 (3) |
| C6| 0.2661 (3) | 0.8058 (2) | 0.91424 (10) | 0.0154 (3) |
| H6A| 0.405015 | 0.802589 | 0.916169 | 0.018* |
| H6B| 0.20699 | 0.78592 | 0.968744 | 0.018* |
| C7| 0.3958 (3) | 0.5088 (2) | 0.90648 (10) | 0.0152 (3) |
| H7A| 0.32656 | 0.482715 | 0.958206 | 0.018* |
| H7B| 0.528732 | 0.510415 | 0.914788 | 0.018* |
| C8| 0.4252 (3) | 0.3788 (2) | 0.85503 (10) | 0.0123 (3) |
| C9| 0.5158 (3) | 0.2141 (2) | 0.88081 (10) | 0.0159 (4) |
| H9| 0.555649 | 0.180246 | 0.93221 | 0.019* |
| C10| 0.5467 (3) | 0.1000 (2) | 0.82986 (11) | 0.0169 (4) |
| H10| 0.610739 | −0.013533 | 0.84539 | 0.02* |
| C11| 0.4830 (3) | 0.1539 (2) | 0.75619 (10) | 0.0153 (3) |
| H11| 0.502104 | 0.078354 | 0.720177 | 0.018* |
| C12| 0.3904 (3) | 0.3211 (2) | 0.73580 (10) | 0.0126 (3) |
| C13| 0.3100 (3) | 0.3899 (2) | 0.65770 (10) | 0.0143 (3) |
| H13A| 0.397572 | 0.323319 | 0.616689 | 0.017* |
| H13B| 0.172891 | 0.385542 | 0.659994 | 0.017* |
| C14| 0.2369 (3) | 0.6343 (2) | 0.55940 (10) | 0.0155 (3) |
| H14A| 0.096005 | 0.640498 | 0.55942 | 0.019* |
| H14B| 0.321889 | 0.562201 | 0.519947 | 0.019* |
| C15| 0.2502 (3) | 0.8035 (2) | 0.53686 (10) | 0.0134 (3) |
| C16| 0.2354 (3) | 0.8748 (2) | 0.45938 (10) | 0.0161 (4) |
| H16| 0.225967 | 0.815293 | 0.420322 | 0.019* |
| C17| 0.2348 (3) | 1.0342 (2) | 0.44024 (11) | 0.0186 (4) |
| H17| 0.225559 | 1.085635 | 0.387808 | 0.022* |
| C18| 0.2479 (3) | 1.1176 (2) | 0.49930 (11) | 0.0197 (4) |
| H18| 0.245914 | 1.227408 | 0.488339 | 0.024* |
### Atomic displacement parameters (Å²)

|     | U¹¹  | U²²  | U³³  | U¹²  | U¹³  | U²³  |
|-----|------|------|------|------|------|------|
| C1  | 0.0158 (9) | 0.0187 (9) | 0.0217 (9) | −0.0080 (7) | −0.0011 (7) | 0.0014 (7) |
| C2  | 0.0147 (9) | 0.0153 (8) | 0.0302 (10) | −0.0057 (7) | 0.0053 (8) | −0.0016 (7) |
| C3  | 0.0187 (10) | 0.0150 (8) | 0.0291 (10) | −0.0080 (7) | 0.0087 (8) | −0.0084 (7) |
| C4  | 0.0159 (9) | 0.0194 (9) | 0.0187 (9) | −0.0077 (7) | 0.0042 (7) | −0.0068 (7) |
| C5  | 0.0121 (9) | 0.0145 (8) | 0.0164 (8) | −0.0062 (7) | 0.0024 (7) | −0.0031 (6) |
| C6  | 0.0184 (9) | 0.0148 (8) | 0.0142 (8) | −0.0053 (7) | −0.0028 (7) | −0.0047 (6) |
| C7  | 0.0179 (9) | 0.0132 (8) | 0.0133 (8) | −0.0039 (7) | −0.0046 (7) | 0.0012 (6) |
| C8  | 0.0109 (8) | 0.0136 (7) | 0.0136 (8) | −0.0062 (6) | −0.0010 (6) | −0.0002 (6) |
| C9  | 0.0164 (9) | 0.0144 (8) | 0.0173 (8) | −0.0061 (7) | −0.0060 (7) | 0.0032 (6) |
| C10 | 0.0135 (9) | 0.0112 (8) | 0.0240 (9) | −0.0035 (7) | −0.0021 (7) | 0.0016 (7) |
| C11 | 0.0147 (9) | 0.0122 (8) | 0.0202 (9) | −0.0061 (7) | 0.0005 (7) | −0.0038 (6) |
| C12 | 0.0099 (8) | 0.0121 (7) | 0.0160 (8) | −0.0043 (6) | −0.0005 (6) | −0.0015 (6) |
| C13 | 0.0180 (9) | 0.0109 (7) | 0.0156 (8) | −0.0059 (7) | −0.0022 (7) | −0.0030 (6) |
| C14 | 0.0199 (9) | 0.0153 (8) | 0.0120 (8) | −0.0060 (7) | −0.0053 (7) | −0.0003 (6) |
| C15 | 0.0100 (8) | 0.0148 (8) | 0.0138 (8) | −0.0028 (6) | −0.0017 (6) | −0.0007 (6) |
| C16 | 0.0129 (9) | 0.0186 (8) | 0.0145 (8) | −0.0030 (7) | −0.0016 (7) | −0.0012 (7) |
| C17 | 0.0116 (9) | 0.0227 (9) | 0.0174 (9) | −0.0045 (7) | −0.0013 (7) | 0.0052 (7) |
| C18 | 0.0141 (9) | 0.0163 (8) | 0.0270 (10) | −0.0057 (7) | −0.0035 (8) | 0.0038 (7) |
| C19 | 0.0147 (9) | 0.0151 (8) | 0.0219 (7) | −0.0062 (7) | −0.0029 (7) | −0.0014 (7) |
| N1  | 0.0113 (7) | 0.0118 (6) | 0.0129 (7) | −0.0042 (5) | −0.0020 (5) | −0.0004 (5) |
| N2  | 0.0147 (8) | 0.0116 (7) | 0.0125 (7) | −0.0044 (6) | −0.0030 (6) | −0.0018 (5) |
| N3  | 0.0153 (8) | 0.0146 (7) | 0.0187 (7) | −0.0069 (6) | 0.0005 (6) | −0.0023 (6) |
| N4  | 0.0155 (8) | 0.0111 (6) | 0.0124 (7) | −0.0049 (6) | −0.0030 (6) | −0.0001 (5) |
| N5  | 0.0146 (8) | 0.0142 (7) | 0.0160 (7) | −0.0065 (6) | −0.0029 (6) | 0.0004 (5) |
| Cl1 | 0.0158 (2) | 0.01449 (19) | 0.0216 (2) | −0.00422 (16) | −0.00132 (17) | 0.00282 (16) |
|        | U11   | U22   | U33   | U12   | U13   | U23   |
|--------|-------|-------|-------|-------|-------|-------|
| Cl2    | 0.0160 (2) | 0.0182 (2) | 0.0178 (2) | −0.00561 (17) | −0.00165 (16) | −0.00182 (16) |
| O1     | 0.0217 (8)  | 0.0225 (7)  | 0.0175 (7)  | −0.0062 (6)   | −0.0017 (6)   | −0.0028 (5)    |
| O2     | 0.0234 (8)  | 0.0193 (7)  | 0.0194 (7)  | −0.0083 (6)   | −0.0002 (6)   | −0.0040 (5)    |

**Geometric parameters (Å, °)**

| Bond/Angle | Value |
|------------|-------|
| C1—N3      | 1.345 (2) |
| C1—C2      | 1.380 (3) |
| C1—H1      | 0.95    |
| C2—C3      | 1.387 (3) |
| C2—H2      | 0.95    |
| C3—C4      | 1.379 (3) |
| C3—H3      | 0.95    |
| C4—C5      | 1.393 (2) |
| C4—H4      | 0.95    |
| C5—N3      | 1.343 (2) |
| C5—C6      | 1.501 (2) |
| C5—C6      | 1.501 (2) |
| C6—N2      | 1.485 (2) |
| C6—H6A     | 0.99    |
| C6—H6B     | 0.99    |
| C7—N2      | 1.488 (2) |
| C7—C8      | 1.507 (2) |
| C7—H7A     | 0.99    |
| C7—H7B     | 0.99    |
| C8—N1      | 1.331 (2) |
| C8—C9      | 1.388 (2) |
| C9—C10     | 1.387 (2) |
| C9—H9      | 0.95    |
| N3—C1—C2   | 123.83 (18) |
| N3—C1—H1   | 118.1   |
| C2—C1—H1   | 118.1   |
| C1—C2—C3   | 118.32 (17) |
| C1—C2—H2   | 120.8   |
| C3—C2—H2   | 120.8   |
| C4—C3—C2   | 118.88 (17) |
| C4—C3—H3   | 120.6   |
| C2—C3—H3   | 120.6   |
| C3—C4—C5   | 119.23 (17) |
| C3—C4—H4   | 120.4   |
| C5—C4—H4   | 120.4   |
| N3—C5—C4   | 122.47 (16) |
| N3—C5—C6   | 119.35 (15) |
### Hydrogen-bond geometry (Å, °)

| D—H···A          | D—H  | H···A  | D···A     | D—H···A |
|------------------|------|-------|-----------|---------|
| O2—H201···Cl2    | 0.85 (3) | 2.41 (3) | 3.1844 (15) | 152 (2) |
| O2—H202···N5     | 0.91 (3) | 2.10 (3) | 2.947 (2)  | 155 (2) |
| N2—H21···O2      | 0.94 (2) | 1.89 (2) | 2.804 (2)  | 165 (2) |
| N2—H22···Cl1\(^i\) | 0.86 (2) | 2.31 (2) | 3.1466 (17)| 152.5 (17) |
| N4—H41···Cl2     | 0.91 (2) | 2.25 (2) | 3.1319 (17)| 164.1 (19) |
| N4—H42···O1\(^i\) | 0.97 (2) | 1.90 (2) | 2.825 (2)  | 158 (2) |
| O1—H101···Cl1    | 0.93 (3) | 2.43 (3) | 3.2611 (15)| 149 (2) |
| O1—H102···N3\(^iv\) | 1.00 (4) | 1.93 (4) | 2.920 (2)  | 172 (3) |
| C3—H3···Cl1\(^iii\) | 0.95 | 2.73 | 3.5702 (19) | 148 |
| C6—H6a···Cl1     | 0.99 | 2.8  | 3.751 (2)  | 161 |
| C7—H7a···Cl1\(^iv\) | 0.99 | 2.78 | 3.7351 (18)| 162 |
| C10—H10···Cl1\(^v\) | 0.95 | 2.71 | 3.6469 (18)| 168 |
| C17—H17···O1\(^vi\) | 0.95 | 2.57 | 3.437 (2)  | 151 |

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