Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{(*E*)-2-Bromo-4-chloro-6-[3-(dimethylammonio)propyliminomethyl]phenolato}dichloridozinc(II)

Li-Juan Ye[a]* and Zhonglu You[b]

[a]Department of Chemistry and Life Sciences, Xiangnan University, Chenzhou 423000, People's Republic of China, and [b]Department of Chemistry, Liaoning Teachers' University, Dalian 116029, People's Republic of China
Correspondence e-mail: lijuan_ye@163.com

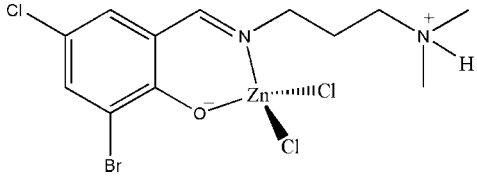
Received 27 May 2008; accepted 29 May 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.049; wR factor = 0.127; data-to-parameter ratio = 19.5.

The title compound, $[ZnCl_2(C_{12}H_{16}BrClN_2O)]$, is a mononuclear zinc(II) complex. The Zn^{II} atom is four-coordinate in a tetrahedral geometry, binding to the phenolate O and imine N atoms of the zwitterionic Schiff base ligand and to two Cl^- ions. In the crystal structure, molecules are linked through intermolecular N—H···Cl hydrogen bonds to form chains running along the *a* axis.

Related literature

For related structures, see: Ali *et al.* (2008); Wang (2007); You (2005). For our recent investigations of metal complex systems, see: Ye & You (2007*a*,*b*,*c*).



Experimental

Crystal data

$[ZnCl_2(C_{12}H_{16}BrClN_2O)]$
M_r = 455.90
Monoclinic, $P2_1/c$
a = 7.522 (4) Å
b = 26.808 (15) Å
c = 8.354 (4) Å
β = 90.921 (9)°
V = 1684.3 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.30 mm^{-1}
T = 298 (2) K
0.32 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.261, T_{max} = 0.275
9470 measured reflections
3633 independent reflections
2283 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.126
S = 1.04
3633 reflections
186 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.931 (4)	Zn1—Cl2	2.2303 (19)
Zn1—N1	1.999 (4)	Zn1—Cl3	2.2489 (19)
O1—Zn1—N1	95.48 (17)	O1—Zn1—Cl3	110.85 (13)
O1—Zn1—Cl2	112.60 (13)	N1—Zn1—Cl3	114.71 (13)
N1—Zn1—Cl2	112.04 (14)	Cl2—Zn1—Cl3	110.45 (8)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···Cl3^{i}	0.91 (5)	2.37 (3)	3.190 (5)	152 (5)

Symmetry code: (i) $x+1, y, z$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Financial support from the Hunan Provincial Natural Sciences Foundation of China (grant No. 03JJY3019) and the Hunan Provincial Educational Ministry Foundation of China (grant No. 05 C627) is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2511).

References

Ali, H. M., Mohamed Mustafa, M. I., Rizal, M. R. & Ng, S. W. (2008). *Acta Cryst.* E**64**, m718–m719.
Bruker (2002). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, S.-X. (2007). *Acta Cryst.* E**63**, m706–m707.
Ye, L.-J. & You, Z. (2007*a*). *Acta Cryst.* E**63**, m523–m525.
Ye, L.-J. & You, Z. (2007*b*). *Acta Cryst.* E**63**, m1837.
Ye, L.-J. & You, Z. (2007*c*). *Acta Cryst.* E**63**, m3137.
You, Z.-L. (2005). *Acta Cryst.* E**61**, m2416–m2418.

supporting information

Acta Cryst. (2008). E**64**, m869 [doi:10.1107/S1600536808016255]

{(*E*)-2-Bromo-4-chloro-6-[3-(dimethylammonio)propyliminomethyl]-phenolato}dichloridozinc(II)

Li-Juan Ye and Zhonglu You

S1. Comment

Recently, we have reported thiocyanate coordinated zinc(II) (Ye & You, 2007*a*), and copper(II) complexes (Ye & You, 2007*b*), and a chlorido-bridged polynuclear copper(II) complex (Ye & You, 2007*c*). As an extension of the work on the crystal structures of such complexes, we report herein the crystal structure of the title compound, (I), Fig. 1.

Compound (I) is a mononuclear zinc(II) complex. The Zn^{II} atom is four-coordinate in a tetrahedral geometry, binding to the phenolate O and imine N atoms of the zwitterionic Schiff base ligand and two Cl^- ions. The coordinate bond values (Table 1) are comparable to those reported in other similar zinc(II) complexes (Wang, 2007; Ali *et al.*, 2008; You, 2005).

In the crystal structure, molecules are linked through intermolecular N–H···Cl hydrogen bonds, Table 2, to form chains running along the *a* axis (Fig. 2).

S2. Experimental

3-Bromo-5-chlorosalicylaldehyde (0.1 mmol, 23.5 mg), *N*,*N*-dimethylpropane-1,3-diamine (0.1 mmol, 10.2 mg), and zinc(II) chloride (0.1 mmol, 13.6 mg) were dissolved in a methanol solution (10 ml). The mixture was stirred at room temperature for 30 min to give a clear colorless solution. Crystals of the compound were formed by slow evaporation of the solvent over a week at room temperature.

S3. Refinement

Atom H2 on the amine N2 atom was located from a difference Fourier map and refined isotropically, with the N–H distance restrained to 0.90 (1) Å, and with U_{iso}(H) fixed at 0.08 Å^2. The remaining H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

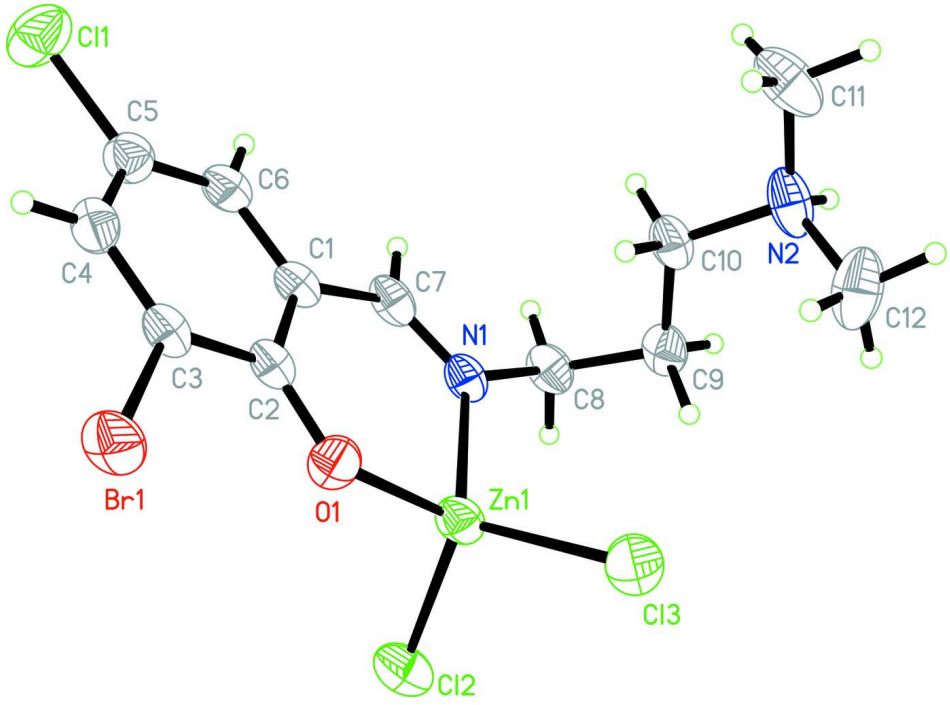


Figure 1

Molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level.

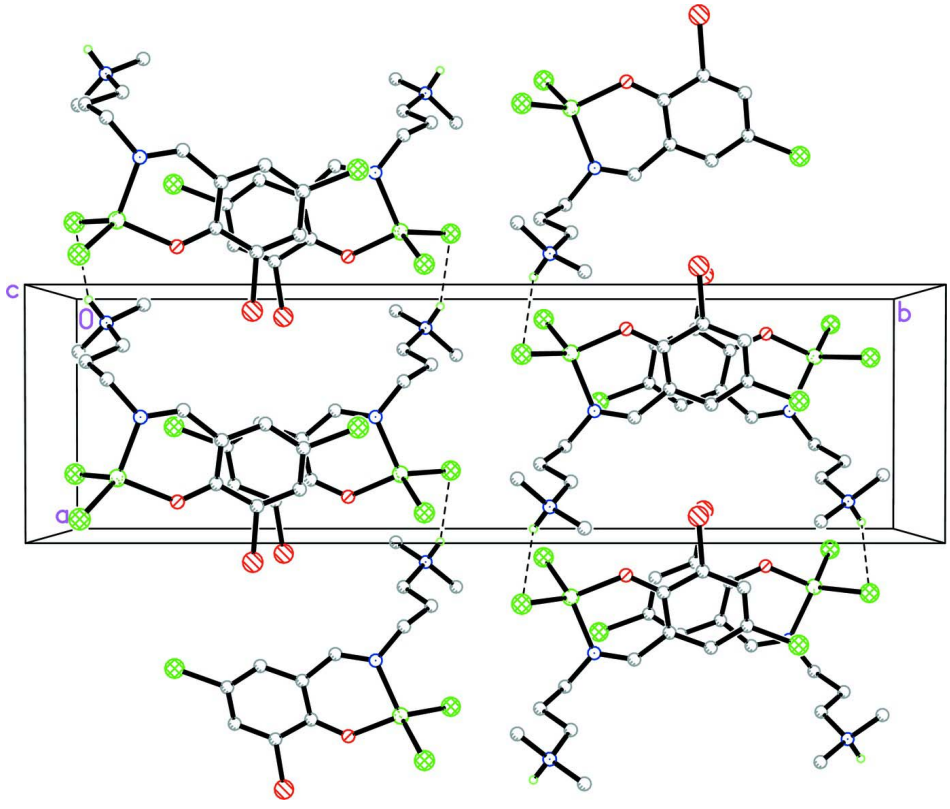


Figure 2

Molecular packing of (I). Intermolecular hydrogen bonds are shown as dashed lines.

{(E)-2-Bromo-4-chloro-6-[3- (dimethylammonio)propyliminomethyl]phenolato}dichloridozinc(II)

Crystal data

$[ZnCl_2(C_{12}H_{16}BrClN_2O)]$
$M_r = 455.90$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.522$ (4) Å
$b = 26.808$ (15) Å
$c = 8.354$ (4) Å
$\beta = 90.921$ (9)°
$V = 1684.3$ (16) Å^3
$Z = 4$
$F(000) = 904$
$D_x = 1.798$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1372 reflections
$\theta = 2.3$–$25.3°$
$\mu = 4.30$ mm^{-1}
$T = 298$ K
Block, colorless
0.32 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.261$, $T_{max} = 0.275$
9470 measured reflections
3633 independent reflections
2283 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.5°$
$h = -9 \rightarrow 9$
$k = -32 \rightarrow 34$
$l = -10 \rightarrow 7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.126$
$S = 1.04$
3633 reflections
186 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 2.1641P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.25129 (8)	0.59843 (2)	0.53367 (8)	0.0531 (2)

Br1	−0.09048 (7)	0.73965 (3)	0.73104 (8)	0.0691 (2)
Cl1	0.4472 (2)	0.86120 (6)	0.5360 (2)	0.0868 (6)
Cl2	0.1025 (2)	0.56893 (7)	0.32087 (19)	0.0748 (5)
Cl3	0.2609 (2)	0.54111 (6)	0.7302 (2)	0.0718 (4)
O1	0.1550 (5)	0.66062 (14)	0.6102 (5)	0.0592 (10)
N1	0.4876 (5)	0.62653 (18)	0.4750 (5)	0.0485 (10)
N2	0.8671 (7)	0.5717 (2)	0.8271 (6)	0.0708 (15)
C1	0.3975 (6)	0.7126 (2)	0.5273 (6)	0.0465 (12)
C2	0.2268 (6)	0.7039 (2)	0.5936 (6)	0.0464 (12)
C3	0.1364 (6)	0.7472 (2)	0.6440 (6)	0.0499 (13)
C4	0.2038 (7)	0.7947 (2)	0.6301 (6)	0.0554 (14)
H4	0.1408	0.8221	0.6675	0.066*
C5	0.3661 (7)	0.8009 (2)	0.5599 (7)	0.0561 (14)
C6	0.4609 (7)	0.7608 (2)	0.5106 (7)	0.0545 (14)
H6	0.5712	0.7658	0.4645	0.065*
C7	0.5140 (6)	0.6730 (2)	0.4739 (6)	0.0501 (13)
H7	0.6226	0.6832	0.4335	0.060*
C8	0.6332 (7)	0.5932 (2)	0.4223 (7)	0.0566 (14)
H8A	0.7281	0.6131	0.3776	0.068*
H8B	0.5886	0.5709	0.3394	0.068*
C9	0.7047 (7)	0.5631 (2)	0.5607 (7)	0.0562 (14)
H9A	0.8007	0.5420	0.5245	0.067*
H9B	0.6115	0.5418	0.6012	0.067*
C10	0.7721 (7)	0.5967 (2)	0.6924 (6)	0.0557 (14)
H10A	0.8515	0.6211	0.6462	0.067*
H10B	0.6717	0.6147	0.7353	0.067*
C11	0.9452 (10)	0.6088 (3)	0.9358 (8)	0.094 (2)
H11A	1.0131	0.6323	0.8755	0.140*
H11B	1.0216	0.5924	1.0125	0.140*
H11C	0.8522	0.6259	0.9906	0.140*
C12	0.7535 (10)	0.5353 (3)	0.9111 (9)	0.092 (2)
H12A	0.8145	0.5236	1.0058	0.137*
H12B	0.7283	0.5075	0.8417	0.137*
H12C	0.6442	0.5510	0.9404	0.137*
H2	0.957 (6)	0.5538 (19)	0.785 (7)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0387 (3)	0.0640 (4)	0.0565 (4)	0.0016 (3)	0.0037 (3)	0.0026 (3)
Br1	0.0423 (3)	0.0841 (5)	0.0814 (5)	0.0067 (3)	0.0171 (3)	−0.0044 (4)
Cl1	0.0821 (12)	0.0638 (10)	0.1152 (15)	−0.0146 (9)	0.0261 (10)	0.0035 (10)
Cl2	0.0598 (9)	0.1019 (13)	0.0625 (10)	−0.0042 (9)	−0.0082 (7)	−0.0015 (9)
Cl3	0.0628 (9)	0.0818 (11)	0.0713 (10)	0.0011 (8)	0.0118 (7)	0.0115 (9)
O1	0.045 (2)	0.056 (2)	0.077 (3)	0.0007 (18)	0.0174 (18)	0.005 (2)
N1	0.033 (2)	0.062 (3)	0.051 (3)	0.009 (2)	0.0019 (18)	0.003 (2)
N2	0.057 (3)	0.095 (4)	0.061 (3)	0.035 (3)	0.007 (2)	0.016 (3)
C1	0.033 (2)	0.064 (3)	0.042 (3)	0.002 (2)	−0.002 (2)	0.001 (3)

C2	0.034 (2)	0.062 (4)	0.043 (3)	0.006 (2)	−0.002 (2)	0.005 (3)
C3	0.036 (3)	0.067 (4)	0.046 (3)	0.006 (2)	0.000 (2)	0.006 (3)
C4	0.056 (3)	0.058 (4)	0.052 (3)	0.009 (3)	−0.004 (3)	−0.001 (3)
C5	0.050 (3)	0.060 (4)	0.058 (4)	−0.002 (3)	0.001 (3)	0.004 (3)
C6	0.039 (3)	0.070 (4)	0.055 (3)	−0.003 (3)	−0.002 (2)	0.004 (3)
C7	0.032 (2)	0.077 (4)	0.041 (3)	0.008 (3)	0.006 (2)	0.008 (3)
C8	0.040 (3)	0.072 (4)	0.058 (4)	0.014 (3)	0.006 (2)	−0.004 (3)
C9	0.040 (3)	0.061 (3)	0.068 (4)	0.014 (3)	0.011 (3)	0.000 (3)
C10	0.041 (3)	0.072 (4)	0.054 (3)	0.011 (3)	0.002 (2)	0.012 (3)
C11	0.081 (5)	0.155 (7)	0.044 (4)	0.008 (5)	−0.010 (3)	−0.003 (4)
C12	0.109 (6)	0.084 (5)	0.083 (5)	0.028 (4)	0.034 (4)	0.031 (4)

Geometric parameters (Å, º)

Zn1—O1	1.931 (4)	C4—H4	0.9300
Zn1—N1	1.999 (4)	C5—C6	1.359 (8)
Zn1—Cl2	2.2303 (19)	C6—H6	0.9300
Zn1—Cl3	2.2489 (19)	C7—H7	0.9300
Br1—C3	1.877 (5)	C8—C9	1.502 (8)
Cl1—C5	1.740 (6)	C8—H8A	0.9700
O1—C2	1.288 (6)	C8—H8B	0.9700
N1—C7	1.261 (7)	C9—C10	1.504 (8)
N1—C8	1.485 (6)	C9—H9A	0.9700
N2—C11	1.464 (9)	C9—H9B	0.9700
N2—C12	1.482 (8)	C10—H10A	0.9700
N2—C10	1.483 (7)	C10—H10B	0.9700
N2—H2	0.91 (5)	C11—H11A	0.9600
C1—C6	1.385 (8)	C11—H11B	0.9600
C1—C2	1.425 (7)	C11—H11C	0.9600
C1—C7	1.451 (7)	C12—H12A	0.9600
C2—C3	1.413 (7)	C12—H12B	0.9600
C3—C4	1.375 (8)	C12—H12C	0.9600
C4—C5	1.372 (8)		
O1—Zn1—N1	95.48 (17)	N1—C7—C1	128.6 (5)
O1—Zn1—Cl2	112.60 (13)	N1—C7—H7	115.7
N1—Zn1—Cl2	112.04 (14)	C1—C7—H7	115.7
O1—Zn1—Cl3	110.85 (13)	N1—C8—C9	110.6 (4)
N1—Zn1—Cl3	114.71 (13)	N1—C8—H8A	109.5
Cl2—Zn1—Cl3	110.45 (8)	C9—C8—H8A	109.5
C2—O1—Zn1	125.6 (3)	N1—C8—H8B	109.5
C7—N1—C8	118.4 (4)	C9—C8—H8B	109.5
C7—N1—Zn1	121.0 (3)	H8A—C8—H8B	108.1
C8—N1—Zn1	120.6 (4)	C8—C9—C10	110.7 (5)
C11—N2—C12	112.5 (6)	C8—C9—H9A	109.5
C11—N2—C10	110.3 (5)	C10—C9—H9A	109.5
C12—N2—C10	112.5 (5)	C8—C9—H9B	109.5
C11—N2—H2	108 (4)	C10—C9—H9B	109.5

C12—N2—H2	106 (4)	H9A—C9—H9B	108.1
C10—N2—H2	107 (4)	N2—C10—C9	115.9 (5)
C6—C1—C2	120.3 (5)	N2—C10—H10A	108.3
C6—C1—C7	116.1 (5)	C9—C10—H10A	108.3
C2—C1—C7	123.6 (5)	N2—C10—H10B	108.3
O1—C2—C3	120.3 (4)	C9—C10—H10B	108.3
O1—C2—C1	124.7 (5)	H10A—C10—H10B	107.4
C3—C2—C1	115.0 (5)	N2—C11—H11A	109.5
C4—C3—C2	123.7 (5)	N2—C11—H11B	109.5
C4—C3—Br1	118.2 (4)	H11A—C11—H11B	109.5
C2—C3—Br1	118.1 (4)	N2—C11—H11C	109.5
C5—C4—C3	118.7 (5)	H11A—C11—H11C	109.5
C5—C4—H4	120.7	H11B—C11—H11C	109.5
C3—C4—H4	120.7	N2—C12—H12A	109.5
C6—C5—C4	120.5 (5)	N2—C12—H12B	109.5
C6—C5—Cl1	121.0 (4)	H12A—C12—H12B	109.5
C4—C5—Cl1	118.5 (5)	N2—C12—H12C	109.5
C5—C6—C1	121.7 (5)	H12A—C12—H12C	109.5
C5—C6—H6	119.2	H12B—C12—H12C	109.5
C1—C6—H6	119.2		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Cl3^{i}	0.91 (5)	2.37 (3)	3.190 (5)	152 (5)

Symmetry code: (i) *x*+1, *y*, *z*.