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cis-Dichloridobis(*N*,*N*,*N*′,*N*′-tetramethylethane-1,2-diamine)platinum(II)

Abdullah M. Asiri,[a,b] Muhammad Nadeem Arshad,[b]* Muhammad Ishaq,[a] Khalid A. Alamry[a,b] and Tanveer Hussain Bokhari[c]*

[a]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203, Jeddah 21589, Saudi Arabia, [b]Center of Excellence for Advanced Materials Research (CEAMR), Faculty of Science, King Abdulaziz University, PO Box 80203, Jeddah 21589, Saudi Arabia, and [c]Department of Chemistry, Government College University, Faisalabad 38000, Pakistan
Correspondence e-mail: mnachemist@hotmail.com, sthbukhari@yahoo.co.uk

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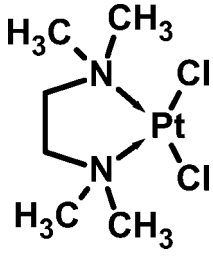
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.010 Å; R factor = 0.044; wR factor = 0.116; data-to-parameter ratio = 19.9.

In the title complex, $[PtCl_2(C_6H_{16}N_2)]$, the Pt^{II} atom adopts a distorted *cis*-PtN_2Cl_2 square-planar coordination geometry. The five-membered chelate ring adopts a twisted conformation. In the crystal, weak C—H···Cl hydrogen bonds link the molecules into (001) sheets.

Related literature

For related structures, see: Abellán-López *et al.* (2012); Boyle *et al.* (2004).



Experimental

Crystal data

$[PtCl_2(C_6H_{16}N_2)]$
M_r = 382.20
Monoclinic, *Ia*
a = 11.8893 (2) Å
b = 6.0207 (1) Å
c = 15.8036 (3) Å
β = 110.549 (2)°
V = 1059.27 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 28.99 mm^{-1}
T = 296 K
0.22 × 0.21 × 0.07 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas, CCD) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.149, T_{max} = 1.000
6899 measured reflections
2091 independent reflections
2067 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
S = 1.03
2091 reflections
105 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.83 e Å^{-3}
$\Delta\rho_{min}$ = −2.02 e Å^{-3}
Absolute structure: Flack (1983), 1005 Friedel pairs
Flack parameter: −0.02 (2)

Table 1
Selected bond lengths (Å).

Pt1—N1	2.071 (7)	Pt1—Cl1	2.292 (4)
Pt1—N2	2.076 (6)	Pt1—Cl2	2.304 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···Cl1^{i}	0.96	2.79	3.724 (8)	166
C4—H4A···Cl1^{ii}	0.97	2.82	3.596 (7)	137

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *X-SEED* (Barbour, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7001).

References

Abellán-López, A., Chicote-Olalla, M. T. & Bautista-Cerezo, D. (2012). *Acta Cryst.* E**68**, m1129.
Agilent (2012). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Boyle, R. C., Mague, J. T. & Fink, M. J. (2004). *Acta Cryst.* E**60**, m40–m41.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2012). E**68**, m1562 [doi:10.1107/S1600536812048295]

cis-Dichloridobis(*N*,*N*,*N*′,*N*′-tetramethylethane-1,2-diamine)platinum(II)

Abdullah M. Asiri, Muhammad Nadeem Arshad, Muhammad Ishaq, Khalid A. Alamry and Tanveer Hussain Bokhari

S1. Comment

The title compound is structurally related with already reported structures of complexes of the type of [MX2(N–N)] (N–N = chelating nitrongen donor ligand) like *cis*-diiodido(*N*,*N*,*N*′,*N*′ -tetramethylethylenediamine-k^2N,N′)palladium(II) (Abellán-López, *et al.* 2012) (II) and cis-dichloro(*N*,*N*,*N*′*N*′-tetramethyl-1,2-diaminoethane) palladium(II) (Boyle *et al.* 2004) (III).

In the structure of molecule I shown in Fig. 1, geometry around the Platinum atom is distorted square planer as N1-Pt1-N2 angle is 84.95 (3)° and Pt to its four co-ordinated atoms distances are [Pt-N = 2.071 (7) Å] and [Pt-Cl = 2.30 (5) Å]. The coordinated ligand atoms and Pt(II) are coplanar with r.m.s. deviation of 0.0119 Å. The planes of the two $N(CH_3)_2$ fragments are twisted at an angle of 12.53(1.05)°. The five membered ring formed by coordination of ligand atoms and metal is nonplaner with r.m.s. deviation of 0.1947 (4)Å and both the halogen atoms (Cl1 & Cl2) are displaced from the least square plane defined by (Pt1/N1/C3/C4/N2) by -0.2216 (1) Å & 0.0425 (1) Å respectively. In the crystal, C—H···Cl interactions link the molecules into (001) sheets (Table 2, Fig. 2).

S2. Experimental

In a round bottom flask took 50 ml of distilled water, 0.5 ml conc. HCL, 0.036 ml of tetramethylethylenediamine (tmeda) (0.24 mmol) and K_2PtCl_4 (0.24 mmol). Refluxed the mixture for about 2 hrs. The solution was changed to pale yellow, it was allowed to cool to room temperature then kept in refrigerator overnight. Pale yellow needles were formed which were filtered, washed with ethanol then with diethylether and dried on vacuum line.

S3. Refinement

All the C—H H-atoms were positioned with idealized geometry with C—H = 0.97 Å for methylene, & C—H = 0.96 Å for methyl groups. H-atoms were refined as riding with U_{iso}(H) = kU_{eq}(C, N), where k = 1.2 for methylene and k = 1.5 for methyl H-atoms.

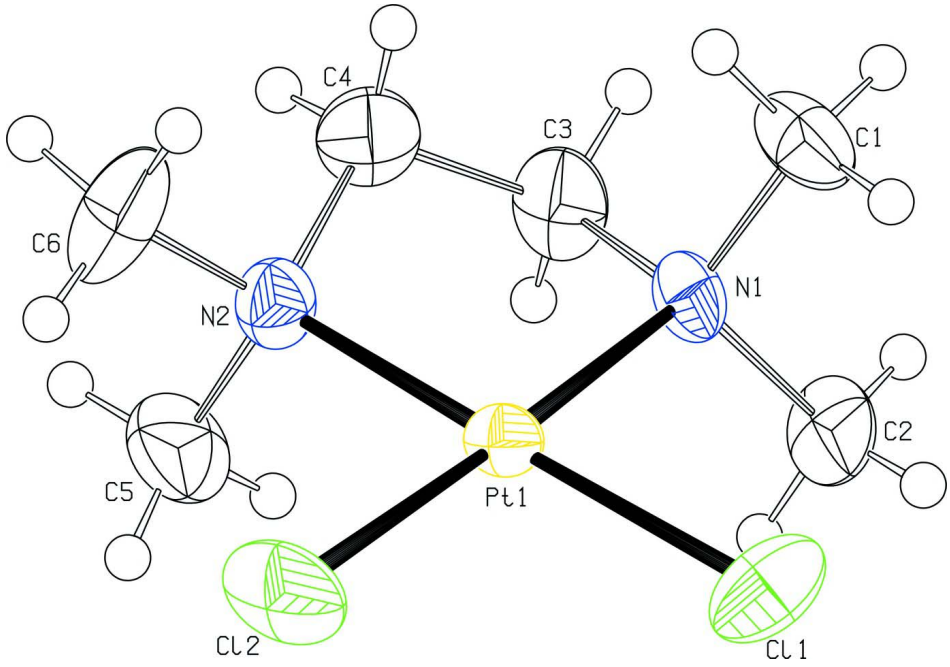

Figure 1

The molecular structure of title complex with 50% probability thermal ellipsoids.

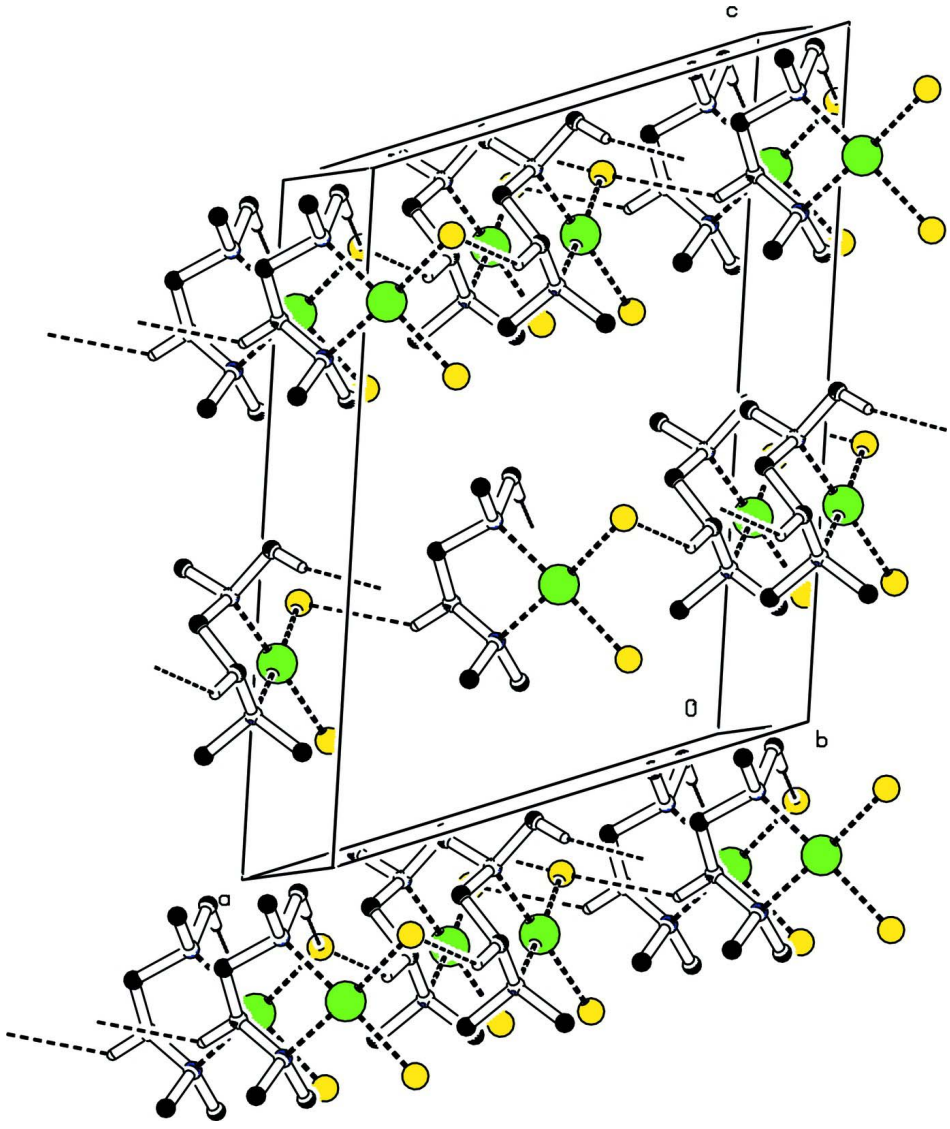

Figure 2

The packing diagram showing hydrogen bonds, drawn using dashed lines. Hydrogen atoms not involved in bonding have been omitted for clarity.

cis-Dichloridobis(*N*,*N*,*N*′,*N*′- tetramethylethane-1,2-diamine)platinum(II)

Crystal data

$[PtCl_2(C_6H_{16}N_2)]$
$M_r = 382.20$
Monoclinic, *Ia*
Hall symbol: I -2ya
$a = 11.8893$ (2) Å
$b = 6.0207$ (1) Å
$c = 15.8036$ (3) Å
$\beta = 110.549$ (2)°
$V = 1059.27$ (3) Å^3
$Z = 4$
$F(000) = 712$
$D_x = 2.397$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 6609 reflections
$\theta = 4.0$–$74.3°$
$\mu = 28.99$ mm^{-1}
$T = 296$ K
Cut needle, yellow
0.22 × 0.21 × 0.07 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas, CCD) diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.149, T_{max} = 1.000
6899 measured reflections
2091 independent reflections
2067 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 74.5°, θ_{min} = 8.0°
h = −14→14
k = −6→7
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
S = 1.03
2091 reflections
105 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.1007P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.83 e Å^{-3}
$\Delta\rho_{min}$ = −2.02 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00105 (13)
Absolute structure: Flack (1983), 1005 Friedel pairs
Absolute structure parameter: −0.02 (2)

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Pt1	0.5018 (3)	0.74348 (4)	0.3050 (2)	0.0267 (2)
Cl1	0.4170 (2)	0.9830 (3)	0.37829 (16)	0.0534 (5)
Cl2	0.3628 (2)	0.8443 (5)	0.16737 (16)	0.0595 (6)
N1	0.6301 (5)	0.6421 (11)	0.4255 (3)	0.0315 (11)
N2	0.5876 (5)	0.5269 (10)	0.2453 (3)	0.0354 (12)
C1	0.5722 (6)	0.5088 (14)	0.4782 (4)	0.0471 (19)
H1A	0.6327	0.4523	0.5318	0.071*
H1B	0.5291	0.3870	0.4420	0.071*
H1C	0.5174	0.6009	0.4949	0.071*
C2	0.6976 (8)	0.828 (2)	0.4835 (5)	0.0472 (18)
H2A	0.6438	0.9147	0.5034	0.071*
H2B	0.7320	0.9203	0.4494	0.071*

H2C	0.7604	0.7687	0.5351	0.071*
C3	0.7209 (7)	0.5022 (14)	0.4027 (4)	0.0481 (18)
H3A	0.7820	0.5970	0.3941	0.058*
H3B	0.7599	0.4007	0.4519	0.058*
C4	0.6581 (7)	0.3734 (14)	0.3176 (5)	0.0483 (16)
H4A	0.7168	0.2957	0.2988	0.058*
H4B	0.6051	0.2640	0.3288	0.058*
C5	0.6643 (9)	0.6529 (18)	0.2053 (6)	0.058 (2)
H5A	0.7253	0.7315	0.2522	0.087*
H5B	0.6157	0.7570	0.1618	0.087*
H5C	0.7014	0.5516	0.1762	0.087*
C6	0.5055 (10)	0.3861 (19)	0.1728 (7)	0.073 (3)
H6A	0.5513	0.2764	0.1549	0.109*
H6B	0.4627	0.4771	0.1218	0.109*
H6C	0.4493	0.3136	0.1948	0.109*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.0225 (3)	0.0267 (3)	0.0262 (3)	−0.0006 (2)	0.00272 (17)	0.00193 (19)
Cl1	0.0403 (8)	0.0435 (11)	0.0769 (11)	0.0024 (7)	0.0214 (8)	−0.0180 (9)
Cl2	0.0491 (9)	0.0623 (17)	0.0450 (8)	0.0031 (10)	−0.0111 (6)	0.0197 (10)
N1	0.027 (2)	0.042 (4)	0.020 (2)	−0.002 (2)	0.001 (2)	0.002 (2)
N2	0.036 (2)	0.039 (3)	0.033 (2)	0.005 (2)	0.014 (2)	−0.001 (2)
C1	0.045 (4)	0.056 (5)	0.033 (3)	−0.009 (3)	0.005 (3)	0.013 (3)
C2	0.044 (4)	0.056 (6)	0.033 (4)	−0.025 (4)	0.003 (3)	−0.013 (4)
C3	0.038 (3)	0.061 (5)	0.036 (3)	0.019 (3)	0.002 (3)	0.003 (3)
C4	0.046 (4)	0.046 (4)	0.050 (4)	0.018 (3)	0.014 (3)	0.005 (3)
C5	0.068 (5)	0.064 (7)	0.057 (4)	0.005 (5)	0.040 (4)	0.010 (4)
C6	0.079 (6)	0.069 (7)	0.065 (5)	0.000 (5)	0.019 (4)	−0.037 (5)

Geometric parameters (Å, º)

Pt1—N1	2.071 (7)	C2—H2B	0.9600
Pt1—N2	2.076 (6)	C2—H2C	0.9600
Pt1—Cl1	2.292 (4)	C3—C4	1.504 (11)
Pt1—Cl2	2.304 (5)	C3—H3A	0.9700
N1—C1	1.488 (7)	C3—H3B	0.9700
N1—C2	1.490 (10)	C4—H4A	0.9700
N1—C3	1.510 (8)	C4—H4B	0.9700
N2—C4	1.480 (9)	C5—H5A	0.9600
N2—C5	1.486 (9)	C5—H5B	0.9600
N2—C6	1.483 (10)	C5—H5C	0.9600
C1—H1A	0.9600	C6—H6A	0.9600
C1—H1B	0.9600	C6—H6B	0.9600
C1—H1C	0.9600	C6—H6C	0.9600
C2—H2A	0.9600		

N1—Pt1—N2	84.9 (3)	N1—C2—H2C	109.5
N1—Pt1—Cl1	91.9 (2)	H2A—C2—H2C	109.5
N2—Pt1—Cl1	176.7 (3)	H2B—C2—H2C	109.5
N1—Pt1—Cl2	177.2 (2)	C4—C3—N1	109.2 (5)
N2—Pt1—Cl2	92.3 (2)	C4—C3—H3A	109.8
Cl1—Pt1—Cl2	90.83 (16)	N1—C3—H3A	109.8
C1—N1—C2	108.4 (5)	C4—C3—H3B	109.8
C1—N1—C3	110.1 (6)	N1—C3—H3B	109.8
C2—N1—C3	106.9 (6)	H3A—C3—H3B	108.3
C1—N1—Pt1	109.7 (4)	N2—C4—C3	109.7 (6)
C2—N1—Pt1	114.1 (6)	N2—C4—H4A	109.7
C3—N1—Pt1	107.6 (3)	C3—C4—H4A	109.7
C4—N2—C5	112.4 (6)	N2—C4—H4B	109.7
C4—N2—C6	106.3 (7)	C3—C4—H4B	109.7
C5—N2—C6	107.4 (6)	H4A—C4—H4B	108.2
C4—N2—Pt1	106.0 (4)	N2—C5—H5A	109.5
C5—N2—Pt1	110.2 (5)	N2—C5—H5B	109.5
C6—N2—Pt1	114.5 (5)	H5A—C5—H5B	109.5
N1—C1—H1A	109.5	N2—C5—H5C	109.5
N1—C1—H1B	109.5	H5A—C5—H5C	109.5
H1A—C1—H1B	109.5	H5B—C5—H5C	109.5
N1—C1—H1C	109.5	N2—C6—H6A	109.5
H1A—C1—H1C	109.5	N2—C6—H6B	109.5
H1B—C1—H1C	109.5	H6A—C6—H6B	109.5
N1—C2—H2A	109.5	N2—C6—H6C	109.5
N1—C2—H2B	109.5	H6A—C6—H6C	109.5
H2A—C2—H2B	109.5	H6B—C6—H6C	109.5

N2—Pt1—N1—C1	−111.5 (5)	Cl1—Pt1—N2—C5	−82 (4)
Cl1—Pt1—N1—C1	69.7 (5)	Cl2—Pt1—N2—C5	77.3 (5)
Cl2—Pt1—N1—C1	−108 (5)	N1—Pt1—N2—C6	135.9 (7)
N2—Pt1—N1—C2	126.6 (4)	Cl1—Pt1—N2—C6	157 (4)
Cl1—Pt1—N1—C2	−52.2 (4)	Cl2—Pt1—N2—C6	−43.9 (7)
Cl2—Pt1—N1—C2	130 (5)	C1—N1—C3—C4	85.3 (7)
N2—Pt1—N1—C3	8.3 (5)	C2—N1—C3—C4	−157.2 (7)
Cl1—Pt1—N1—C3	−170.5 (5)	Pt1—N1—C3—C4	−34.3 (8)
Cl2—Pt1—N1—C3	11 (5)	C5—N2—C4—C3	76.8 (8)
N1—Pt1—N2—C4	19.1 (5)	C6—N2—C4—C3	−165.9 (6)
Cl1—Pt1—N2—C4	40 (4)	Pt1—N2—C4—C3	−43.7 (7)
Cl2—Pt1—N2—C4	−160.7 (5)	N1—C3—C4—N2	53.2 (8)
N1—Pt1—N2—C5	−102.8 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···Cl1^{i}	0.96	2.79	3.724 (8)	166

C4—H4*A*···Cl1^{ii}	0.97	2.82	3.596 (7)	137

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