Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloro-*N*-[4-chloro-2-(2-chlorobenzoyl)phenyl]acetamide

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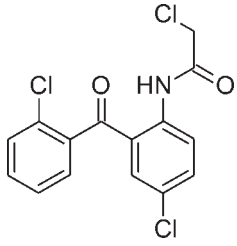
Received 22 January 2010; accepted 27 January 2010

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.113; data-to-parameter ratio = 12.7.

In the title compound, $C_{15}H_{10}Cl_3NO_2$, an intramolecular N—H···O hydrogen bond forms a six-membered ring and enforces an almost coplanar conformation for the acetamido group, the central benzene ring and the bridging carbonyl C—C(=O)—C group: the dihedral angles between the benzene ring and the acetamide and carbonyl C—C(=O)—C planes are 7.06 (11) and 7.17 (12)°, respectively. The dihedral angle between the two benzene rings is 67.43 (9)°. Because a strong hydrogen-bond donor is involved in the intramolecular interaction, the crystal packing is determined by weak C—H···O and C—H···Cl interactions.

Related literature

The title compound is isostructural with 2-chloroacetamido-5-chloro-2′-fluorobenzophenone (Prasanna & Guru Row, 2000). For the isostructurality index, see: Kálmán *et al.* (1991); Kubicki & Szafrański (1998). For a related structure, see: Malathy Sony *et al.* (2005). For the biological activity of benzophenone derivatives, see: Evans *et al.* (1987). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$C_{15}H_{10}Cl_3NO_2$
M_r = 342.59
Triclinic, $P\overline{1}$
a = 7.5776 (9) Å
b = 10.1565 (10) Å
c = 10.7862 (12) Å
α = 70.069 (8)°
β = 77.604 (9)°
γ = 70.388 (8)°
V = 730.47 (14) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 5.71 mm^{-1}
T = 295 K
0.35 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction SuperNova (single source at offset) Atlas diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.117, T_{max} = 0.319
5245 measured reflections
2917 independent reflections
2610 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 1.05
2917 reflections
230 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8···O1	0.84 (3)	1.95 (3)	2.634 (2)	138 (3)
C6—H6···Cl14^{i}	0.94 (3)	2.87 (3)	3.675 (2)	143 (2)
C11—H11*B*···O10^{ii}	0.93 (3)	2.50 (3)	3.320 (3)	147 (2)
C18—H18···Cl14^{iii}	0.95 (3)	2.84 (3)	3.745 (3)	161 (2)

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Stereochemical Workstation Operation Manual* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

BPS thanks R. L. FineChem, Bangalore, India, for the gift of a sample of the title compound.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2519).

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supporting information

Acta Cryst. (2010). E**66**, o499 [https://doi.org/10.1107/S1600536810003375]

2-Chloro-*N*-[4-chloro-2-(2-chlorobenzoyl)phenyl]acetamide

Grzegorz Dutkiewicz, B. P. Siddaraju, H. S. Yathirajan, B. Narayana and Maciej Kubicki

S1. Comment

Benzophenone and related compounds have been reported to act as e.g., antiallergic, anti-inflammatory, antiasthmatic, antimalarial, anti-microbial and antianaphylactic agents (Evans *et al.*, 1987). Here we report the crystal structure of 2-chloroacetamido-5-chloro-2′-chlorobenzophenone (alternative name: 2-chloro-*N*-{4-chloro-2-[(2-chlorophenyl)-carbonyl]phenyl}acetamide; **1**, Scheme 1), which is an intermediate in the synthesis of certain anxiolytic, anticonvulsant and sedative drugs, and is also a starting material for the synthesis of diazepam and other benzodiazepines.

The structure of **1** is isostructural with the previously described 2-chloroacetamido-5-chloro-2′-fluorobenzophenone derivative (Prasanna & Guru Row, 2000). Both compounds crystallize in the triclinic P-1 space group, and the unit cell dimensions are similar. Also the positions of the atoms in the unit cell are similar, after applying the transformation (index 1 refers to Prasanna & Guru Row, 2 - to the present structure): $x_2=x_1+0.5$, $y_2=y_1+0.5$, $z_2=z_1+1.5$. The isostructurality index (Kálmán *et al.*, 1991), which describes the differences between the positions of the atoms in the unit cell has the value of 97.4% (for perfect isostructurality it should be 100%). Kubicki & Szafrański (1998) proposed the modification of this latter parameter which takes into account the point group symmetry and gives more absolute measure of the degree of isostructurality: it should be 1 for ideally isomorphous compounds and 0 for randomly distributed atoms. The value of this modified index is 0.94.

The conformation of **1** (Fig. 1) might be described by dihedral angles between four approximately planar fragments: acetamide [A, planar within 0.0065 (19) Å, with Cl2 atom significantly, by 0.110 (5)Å out of the plane], central phenyl [B, maximum deviation 0.0034 (14) Å], bridging carbonyl group C—C(=O)-C [C, max. deviation 0.015 (2) Å], and terminal phenyl [D, 0.0045 (19) Å]. The first three are close to coplanarity, the dihedral angles are A/B 7.06 (11)° and B/C 7.17 (12)°. Such a coplanar conformation of phenyl and carbonyl plane is quite uncommon for benzophenones, in a majority of the compounds found in the CSD (Allen, 2002) both phenyl rings are almost equally, and significantly, twisted with respect to the central plane. In the case of **1**, as in some similar cases (for instance in the isostructural 2′-fluoro derivative but also in two crystal forms of 2-chloroacetamido-5-chlorobenzophenone (monoclinic: Prasanna & Guru Row, 2000, and triclinic: Malathy Sony *et al.*, 2005), the factor responsible for such a coplanar conformation is the intramolecular hydrogen bond N—H···O (cf. Table 1). This hydrogen bond closes the six-membered ring, planar within 0.072 (7) Å. The second phenyl ring, which has no factor that can stabilize coplanar conformation, is typically, by 62.14 (10)°, twisted with respect to the bridge. The Cl atom of chloroacetamide group is anti with respect to the oxygen atom [O10—C9—C11—Cl12 torsion angle of 176.4 (2)°] and syn with respect to the N atom [N8—C9—C11—Cl12 is -4.8 (3)°]

In the crystal structure there are some weak C—H···O and C—H···Cl interactions, which might be of some importance when the strong hydrogen bond donor is involved in intramolecular interaction (Fig. 2)

S2. Experimental

The title compound was obtained as a gift sample from R. L. FineChem, Bangalore, India. The compound was used without further purification. X-ray quality crystals were obtained by slow evaporation from ethyl acetate solution (m.p. 436-438 K).

S3. Refinement

Hydrogen atoms were found in the subsequent difference Fourier maps, and freely refined.

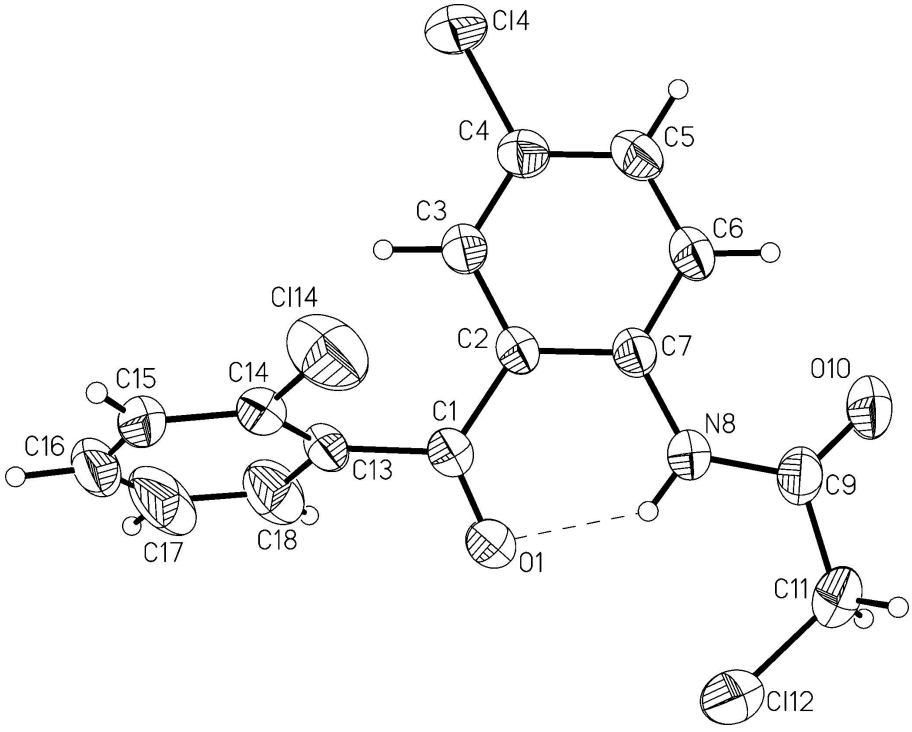

Figure 1

Anisotropic ellipsoid representation of the title compound together with atom labelling scheme. The ellipsoids are drawn at 50% probability level, hydrogen atoms are depicted as spheres with arbitrary radii. The intramolecular hydrogen bond is shown as a dashed line.

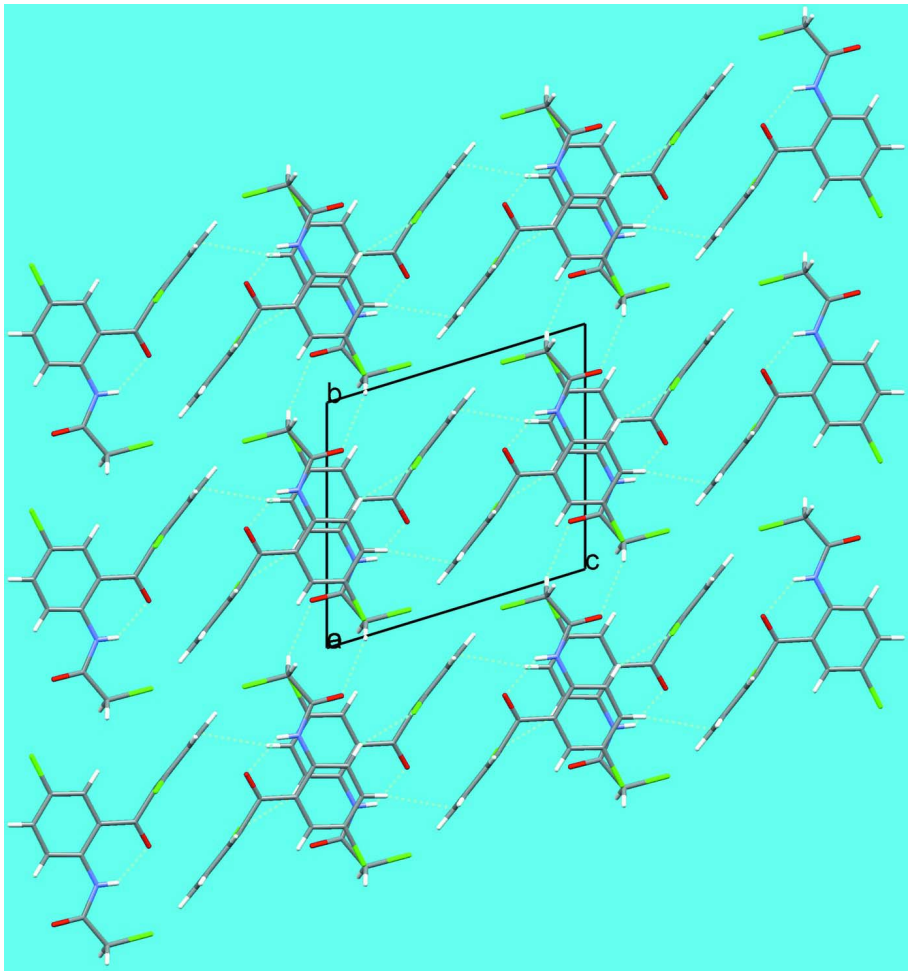

Figure 2

The crystal packing of the title compound, as seen along the *a* axis. Hydrogen bonds are shown as dashed lines.

2-Chloro-*N*-[4-chloro-2-(2-chlorobenzoyl)phenyl]acetamide

Crystal data

$C_{15}H_{10}Cl_3NO_2$
$M_r = 342.59$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.5776\ (9)$ Å
$b = 10.1565\ (10)$ Å
$c = 10.7862\ (12)$ Å
$\alpha = 70.069\ (8)°$
$\beta = 77.604\ (9)°$
$\gamma = 70.388\ (8)°$
$V = 730.47\ (14)$ Å^3
$Z = 2$
$F(000) = 348$
$D_x = 1.558$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 3832 reflections
$\theta = 4.4–75.1°$
$\mu = 5.71$ mm^{-1}
$T = 295$ K
Prism, pink
0.35 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction SuperNova (single source at offset) Atlas diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator

Detector resolution: 10.5357 pixels mm^{-1}
ω–scan
Absorption correction: multi-scan
(*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.117, T_{max} = 0.319
5245 measured reflections
2917 independent reflections
2610 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 75.2°, θ_{min} = 4.4°
h = −9→9
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 1.05
2917 reflections
230 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2 + 0.3949P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 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.

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 $F^2 > 2\sigma(F^2)$ 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}
C1	0.2330 (3)	0.4690 (2)	0.74281 (19)	0.0407 (4)
O1	0.1250 (3)	0.58486 (19)	0.68930 (16)	0.0679 (5)
C2	0.2780 (3)	0.4324 (2)	0.87982 (17)	0.0347 (4)
C3	0.3816 (3)	0.2896 (2)	0.94118 (19)	0.0391 (4)
H3	0.422 (3)	0.219 (2)	0.889 (2)	0.043 (6)*
C4	0.4253 (3)	0.2515 (2)	1.06806 (19)	0.0419 (4)
Cl4	0.55643 (9)	0.07373 (6)	1.14246 (6)	0.05951 (19)
C5	0.3676 (3)	0.3534 (2)	1.1378 (2)	0.0482 (5)
H5	0.393 (4)	0.325 (3)	1.228 (3)	0.074 (9)*
C6	0.2645 (3)	0.4939 (2)	1.0804 (2)	0.0454 (5)
H6	0.230 (4)	0.562 (3)	1.129 (3)	0.059 (7)*
C7	0.2178 (3)	0.5364 (2)	0.95170 (18)	0.0358 (4)
N8	0.1173 (3)	0.67993 (18)	0.88973 (17)	0.0415 (4)
H8	0.094 (4)	0.696 (3)	0.812 (3)	0.067 (8)*
C9	0.0393 (3)	0.7935 (2)	0.9426 (2)	0.0448 (5)
O10	0.0375 (3)	0.78715 (18)	1.05679 (17)	0.0650 (5)
C11	−0.0562 (4)	0.9388 (3)	0.8497 (3)	0.0545 (6)
H11B	−0.006 (4)	1.010 (3)	0.851 (3)	0.066 (8)*
H11A	−0.189 (5)	0.970 (4)	0.878 (3)	0.083 (10)*

Cl12	−0.03818 (13)	0.94573 (7)	0.68136 (7)	0.0826 (3)
C13	0.3127 (3)	0.3605 (2)	0.66429 (18)	0.0403 (4)
C14	0.5017 (3)	0.3148 (2)	0.61956 (19)	0.0465 (5)
Cl14	0.66554 (9)	0.37077 (10)	0.66357 (7)	0.0759 (2)
C15	0.5645 (5)	0.2289 (3)	0.5339 (2)	0.0701 (9)
H15	0.693 (6)	0.200 (4)	0.509 (4)	0.102 (12)*
C16	0.4381 (7)	0.1877 (3)	0.4935 (3)	0.0855 (12)
H16	0.478 (5)	0.129 (4)	0.433 (4)	0.109 (12)*
C17	0.2507 (8)	0.2312 (4)	0.5360 (3)	0.0885 (12)
H17	0.162 (6)	0.198 (4)	0.511 (4)	0.110 (13)*
C18	0.1858 (5)	0.3185 (3)	0.6211 (3)	0.0646 (7)
H18	0.054 (4)	0.345 (3)	0.647 (3)	0.064 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0457 (11)	0.0416 (10)	0.0345 (9)	−0.0059 (8)	−0.0076 (8)	−0.0154 (8)
O1	0.0874 (13)	0.0584 (10)	0.0450 (9)	0.0187 (9)	−0.0284 (8)	−0.0254 (8)
C2	0.0395 (9)	0.0372 (9)	0.0292 (8)	−0.0102 (8)	−0.0037 (7)	−0.0129 (7)
C3	0.0472 (11)	0.0362 (9)	0.0353 (9)	−0.0107 (8)	−0.0050 (8)	−0.0129 (8)
C4	0.0495 (11)	0.0382 (10)	0.0356 (9)	−0.0121 (8)	−0.0076 (8)	−0.0065 (8)
Cl4	0.0745 (4)	0.0419 (3)	0.0526 (3)	−0.0059 (3)	−0.0225 (3)	−0.0034 (2)
C5	0.0644 (14)	0.0501 (12)	0.0308 (9)	−0.0150 (10)	−0.0110 (9)	−0.0105 (9)
C6	0.0595 (13)	0.0464 (11)	0.0339 (10)	−0.0124 (9)	−0.0062 (9)	−0.0185 (9)
C7	0.0415 (10)	0.0362 (9)	0.0319 (9)	−0.0112 (8)	−0.0031 (7)	−0.0132 (7)
N8	0.0518 (10)	0.0364 (8)	0.0364 (9)	−0.0057 (7)	−0.0076 (7)	−0.0161 (7)
C9	0.0521 (12)	0.0401 (10)	0.0465 (11)	−0.0124 (9)	−0.0024 (9)	−0.0205 (9)
O10	0.0977 (14)	0.0495 (9)	0.0508 (9)	−0.0098 (9)	−0.0101 (9)	−0.0283 (8)
C11	0.0611 (15)	0.0390 (11)	0.0633 (14)	−0.0044 (10)	−0.0096 (12)	−0.0231 (10)
Cl12	0.1198 (6)	0.0491 (3)	0.0563 (4)	0.0106 (4)	−0.0247 (4)	−0.0128 (3)
C13	0.0556 (12)	0.0394 (10)	0.0296 (9)	−0.0123 (9)	−0.0095 (8)	−0.0129 (7)
C14	0.0579 (12)	0.0412 (10)	0.0317 (9)	0.0000 (9)	−0.0095 (9)	−0.0111 (8)
Cl14	0.0489 (3)	0.1181 (6)	0.0624 (4)	−0.0212 (4)	−0.0057 (3)	−0.0312 (4)
C15	0.101 (2)	0.0478 (13)	0.0343 (11)	0.0192 (14)	−0.0117 (13)	−0.0156 (10)
C16	0.172 (4)	0.0390 (12)	0.0384 (13)	−0.0081 (17)	−0.0247 (18)	−0.0161 (10)
C17	0.171 (4)	0.074 (2)	0.0541 (16)	−0.064 (2)	−0.033 (2)	−0.0190 (15)
C18	0.0825 (19)	0.0759 (17)	0.0535 (14)	−0.0381 (15)	−0.0126 (13)	−0.0231 (13)

Geometric parameters (Å, º)

C1—O1	1.217 (3)	C9—O10	1.209 (3)
C1—C2	1.482 (2)	C9—C11	1.514 (3)
C1—C13	1.506 (3)	C11—Cl12	1.770 (3)
C2—C3	1.401 (3)	C11—H11B	0.93 (3)
C2—C7	1.417 (2)	C11—H11A	0.96 (3)
C3—C4	1.371 (3)	C13—C14	1.381 (3)
C3—H3	0.99 (2)	C13—C18	1.388 (3)
C4—C5	1.383 (3)	C14—C15	1.387 (3)

C4—Cl4	1.744 (2)	C14—Cl14	1.732 (2)
C5—C6	1.374 (3)	C15—C16	1.363 (5)
C5—H5	0.96 (3)	C15—H15	0.92 (4)
C6—C7	1.392 (3)	C16—C17	1.363 (6)
C6—H6	0.94 (3)	C16—H16	0.97 (4)
C7—N8	1.401 (3)	C17—C18	1.392 (4)
N8—C9	1.361 (3)	C17—H17	0.96 (4)
N8—H8	0.84 (3)	C18—H18	0.95 (3)

O1—C1—C2	122.49 (17)	N8—C9—C11	116.46 (19)
O1—C1—C13	116.25 (17)	C9—C11—Cl12	116.35 (15)
C2—C1—C13	121.21 (17)	C9—C11—H11B	109.2 (18)
C3—C2—C7	118.78 (17)	Cl12—C11—H11B	106.8 (18)
C3—C2—C1	118.91 (16)	C9—C11—H11A	111 (2)
C7—C2—C1	122.30 (17)	Cl12—C11—H11A	106 (2)
C4—C3—C2	120.57 (18)	H11B—C11—H11A	107 (3)
C4—C3—H3	122.2 (13)	C14—C13—C18	118.3 (2)
C2—C3—H3	117.3 (13)	C14—C13—C1	123.67 (19)
C3—C4—C5	120.60 (19)	C18—C13—C1	117.5 (2)
C3—C4—Cl4	120.01 (16)	C13—C14—C15	121.3 (3)
C5—C4—Cl4	119.38 (16)	C13—C14—Cl14	120.50 (15)
C6—C5—C4	120.02 (19)	C15—C14—Cl14	118.2 (2)
C6—C5—H5	119.4 (18)	C16—C15—C14	119.6 (3)
C4—C5—H5	120.5 (18)	C16—C15—H15	123 (2)
C5—C6—C7	120.93 (19)	C14—C15—H15	117 (2)
C5—C6—H6	118.3 (16)	C15—C16—C17	120.4 (2)
C7—C6—H6	120.8 (16)	C15—C16—H16	121 (2)
C6—C7—N8	121.99 (17)	C17—C16—H16	118 (2)
C6—C7—C2	119.09 (18)	C16—C17—C18	120.6 (3)
N8—C7—C2	118.90 (16)	C16—C17—H17	121 (2)
C9—N8—C7	128.23 (18)	C18—C17—H17	119 (3)
C9—N8—H8	116 (2)	C13—C18—C17	119.9 (3)
C7—N8—H8	116 (2)	C13—C18—H18	123.9 (17)
O10—C9—N8	125.6 (2)	C17—C18—H18	116.2 (17)
O10—C9—C11	117.95 (19)		

O1—C1—C2—C3	170.9 (2)	C7—N8—C9—O10	−3.3 (4)
C13—C1—C2—C3	−6.2 (3)	C7—N8—C9—C11	178.0 (2)
O1—C1—C2—C7	−8.3 (3)	O10—C9—C11—Cl12	176.4 (2)
C13—C1—C2—C7	174.60 (18)	N8—C9—C11—Cl12	−4.8 (3)
C7—C2—C3—C4	−0.6 (3)	O1—C1—C13—C14	114.9 (2)
C1—C2—C3—C4	−179.76 (19)	C2—C1—C13—C14	−67.8 (3)
C2—C3—C4—C5	0.1 (3)	O1—C1—C13—C18	−56.9 (3)
C2—C3—C4—Cl4	−179.37 (15)	C2—C1—C13—C18	120.4 (2)
C3—C4—C5—C6	0.4 (4)	C18—C13—C14—C15	−0.2 (3)
Cl4—C4—C5—C6	179.89 (18)	C1—C13—C14—C15	−171.9 (2)
C4—C5—C6—C7	−0.5 (4)	C18—C13—C14—Cl14	176.90 (18)
C5—C6—C7—N8	−178.2 (2)	C1—C13—C14—Cl14	5.2 (3)

C5—C6—C7—C2	0.1 (3)	C13—C14—C15—C16	−0.4 (3)
C3—C2—C7—C6	0.4 (3)	Cl14—C14—C15—C16	−177.56 (19)
C1—C2—C7—C6	179.63 (19)	C14—C15—C16—C17	0.5 (4)
C3—C2—C7—N8	178.80 (18)	C15—C16—C17—C18	0.1 (5)
C1—C2—C7—N8	−2.0 (3)	C14—C13—C18—C17	0.7 (4)
C6—C7—N8—C9	−5.3 (3)	C1—C13—C18—C17	172.9 (2)
C2—C7—N8—C9	176.4 (2)	C16—C17—C18—C13	−0.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N8—H8···O1	0.84 (3)	1.95 (3)	2.634 (2)	138 (3)
C6—H6···Cl14^{i}	0.94 (3)	2.87 (3)	3.675 (2)	143 (2)
C11—H11*B*···O10^{ii}	0.93 (3)	2.50 (3)	3.320 (3)	147 (2)
C18—H18···Cl14^{iii}	0.95 (3)	2.84 (3)	3.745 (3)	161 (2)

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