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2-Chloro-*N*-(3-methylphenyl)acetamide

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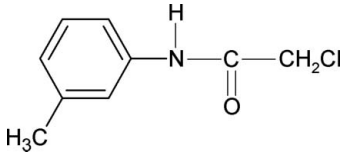
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.136; data-to-parameter ratio = 14.5.

The conformation of the N—H bond in the structure of the title compound, $C_9H_{10}ClNO$, is *syn* to the *meta*-methyl group, in contrast to the *anti* conformation observed with respect to the *meta*-nitro group in 2-chloro-*N*-(3-nitrophenyl)acetamide. The asymmetric unit of the title compound contains two molecules. The geometric parameters of the title compound are similar to those of 2-chloro-*N*-(4-methylphenyl)acetamide, 2-chloro-*N*-(3-nitrophenyl)acetamide and other acetanilides. Dual intermolecular N—H···O hydrogen bonds link the molecules in the direction of the *a* axis.

Related literature

For related literature, see: Gowda *et al.* (2006, 2007*a*,*b*,*c*).



Experimental

Crystal data

$C_9H_{10}ClNO$
M_r = 183.63
Triclinic, $P\overline{1}$
a = 8.326 (3) Å
b = 9.742 (3) Å
c = 11.491 (4) Å
α = 91.21 (1)°
β = 97.97 (1)°
γ = 98.08 (1)°
V = 913.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 299 (2) K
0.75 × 0.45 × 0.17 mm

Data collection

Stoe STADI-4 four-circle diffractometer
Absorption correction: ψ-scan (North *et al.*, 1968)
T_{min} = 0.704, T_{max} = 0.918
3214 measured reflections
3214 independent reflections
2651 reflections with $I > 2\sigma(I)$
3 standard reflections
frequency: 180 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.136
S = 1.05
3214 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.04	2.891 (2)	171
N2—H2···O1	0.86	2.13	2.970 (2)	166

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

Data collection: *STADI4* (Stoe & Cie, 1987); cell refinement: *STADI4*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2289).

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supporting information

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2-Chloro-*N*-(3-methylphenyl)acetamide

B. Thimme Gowda, Ingrid Svoboda, Sabine Foro, Shi-qi Dou and Hartmut Fuess

S1. Comment

In the present work, the structure of 2-chloro-*N*-(3-methylphenyl)- acetamide (3MPCA) has been determined as part of a study of the effect of ring and side chain substitutions on the solid state geometry of aromatic amides (Gowda *et al.*, 2007*a*, 2007*b*, 2007*c*). The conformation of the N—H bond in the structure of 3MPCA is *syn* to the *meta* methyl group, in contrast to the *anti* conformation observed with respect to the *meta* nitro group in the 2-chloro-*N*-(3-nitrophenyl)-acetamide (3NPCA)(Gowda *et al.*, 2007*b*). The asymmetric unit of 3MPCA crystal contains two molecules. The geometric parameters of 3MPCA are similar to those of 3NPCA (Gowda *et al.*, 2007*b*), 2-chloro-*N*-(4-methylphenyl)-acetamide (Gowda *et al.*, 2007*a*), 2-chloro-*N*- (2-chlorophenyl)-acetamide (Gowda *et al.*, 2007*c*) and other acetanilides. The molecules in 3MPcA are linked into infinite diagonal chains through dual intermolecular N1—H1···O2 and N2—H2—O1 hydrogen bonding in the *bc* plane (Table 1 and Fig.2).

S2. Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2006). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2006). Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

S3. Refinement

The H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH_3) or 0.97 Å (CH_2Cl) and N—H = 0.86 Å with U_{iso}(H) = 1.2 U_{eq}(CH or NH) and U_{iso}(H) = 1.4 U_{eq}(CH_3).

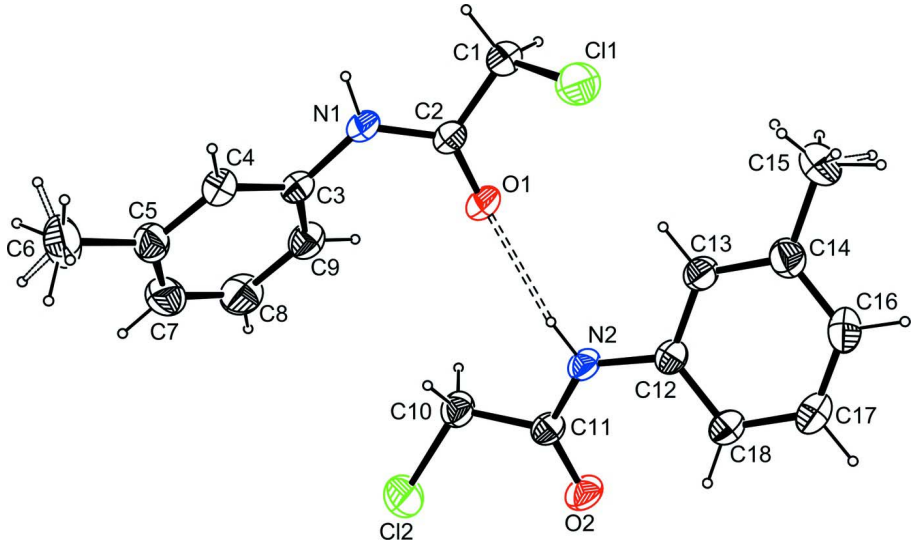

Figure 1

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. H bond is shown as dashed line.

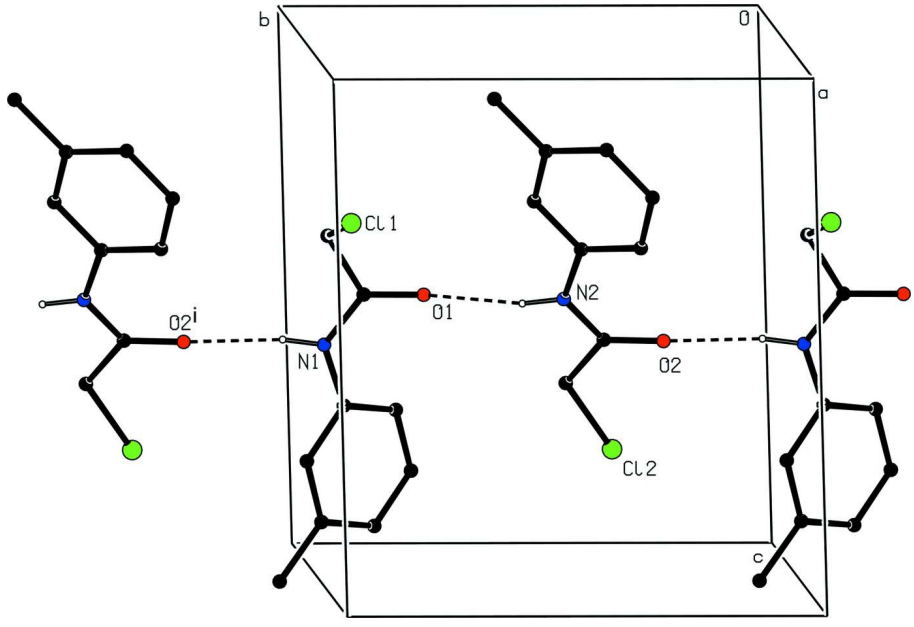

Figure 2

Partial packing view showing the formation of the chain through N—H···O hydrogen bondings. H atoms not involved in H bonds have been omitted for clarity. H bonds are shown as dashed lines. [Symmetry code: (i) x, $y+1$, z]

2-Chloro-*N*-(3-methylphenyl)acetamide

Crystal data

$C_9H_{10}ClNO$
$M_r = 183.63$
Triclinic, $P\overline{1}$
Hall symbol: -P 1

$a = 8.326\ (3)$ Å
$b = 9.742\ (3)$ Å
$c = 11.491\ (4)$ Å
$\alpha = 91.21\ (1)°$

β = 97.97 (1)°
γ = 98.08 (1)°
V = 913.1 (5) Å^3
Z = 4
F(000) = 384
D_x = 1.336 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 88 reflections
θ = 18.0–22.6°
μ = 0.37 mm^{-1}
T = 299 K
Flat prism, colourless
0.75 × 0.45 × 0.17 mm

Data collection

Stoe STADI-4 four-circle diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Profile fitted scans 2θ/ω=1/1
Absorption correction: empirical (using intensity measurements) (North *et al.*, 1968)
T_{min} = 0.704, T_{max} = 0.918
3214 measured reflections

3214 independent reflections
2651 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −9→9
k = −11→11
l = 0→13
3 standard reflections every 180 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.136
S = 1.05
3214 reflections
221 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
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 0.2235P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 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}	Occ. (<1)
Cl1	0.38090 (9)	0.90157 (7)	0.35203 (6)	0.0807 (3)	
C1	0.1956 (3)	0.9307 (2)	0.40069 (18)	0.0552 (5)	
H1A	0.1966	1.0295	0.4143	0.066*	
H1B	0.1039	0.8970	0.3406	0.066*	
C2	0.1756 (2)	0.85664 (19)	0.51299 (17)	0.0451 (4)	
O1	0.16114 (19)	0.72994 (13)	0.51555 (13)	0.0570 (4)	
N1	0.1734 (2)	0.94148 (15)	0.60666 (14)	0.0464 (4)	
H1	0.1852	1.0290	0.5951	0.056*	

C3	0.1537 (2)	0.90157 (18)	0.72263 (17)	0.0444 (4)	
C4	0.2336 (2)	0.9904 (2)	0.81524 (18)	0.0518 (5)	
H4	0.3003	1.0708	0.7996	0.062*	
C5	0.2157 (3)	0.9613 (2)	0.93068 (19)	0.0606 (6)	
C6	0.3022 (4)	1.0612 (4)	1.0296 (2)	0.0896 (9)	
H6A	0.2223	1.0971	1.0698	0.108*	0.56 (3)
H6B	0.3678	1.1364	0.9980	0.108*	0.56 (3)
H6C	0.3712	1.0136	1.0838	0.108*	0.56 (3)
H6D	0.4186	1.0676	1.0313	0.108*	0.44 (3)
H6E	0.2730	1.0283	1.1031	0.108*	0.44 (3)
H6F	0.2697	1.1511	1.0173	0.108*	0.44 (3)
C7	0.1180 (3)	0.8405 (3)	0.9516 (2)	0.0731 (7)	
H7	0.1062	0.8182	1.0286	0.088*	
C8	0.0373 (3)	0.7520 (3)	0.8598 (2)	0.0752 (7)	
H8	−0.0283	0.6711	0.8757	0.090*	
C9	0.0528 (3)	0.7821 (2)	0.7446 (2)	0.0561 (5)	
H9	−0.0034	0.7233	0.6830	0.067*	
Cl2	0.11737 (11)	0.34078 (8)	0.80955 (6)	0.0934 (3)	
C10	0.1373 (3)	0.4359 (2)	0.68356 (19)	0.0552 (5)	
H10A	0.0296	0.4534	0.6483	0.066*	
H10B	0.2035	0.5250	0.7063	0.066*	
C11	0.2149 (2)	0.36313 (18)	0.59258 (17)	0.0458 (4)	
O2	0.2274 (2)	0.24012 (14)	0.59346 (14)	0.0646 (4)	
N2	0.26143 (19)	0.44939 (15)	0.51024 (14)	0.0449 (4)	
H2	0.2476	0.5344	0.5204	0.054*	
C12	0.3306 (2)	0.41834 (18)	0.40855 (16)	0.0429 (4)	
C13	0.3227 (2)	0.5128 (2)	0.31995 (18)	0.0508 (5)	
H13	0.2722	0.5908	0.3293	0.061*	
C14	0.3889 (3)	0.4929 (2)	0.21770 (19)	0.0608 (5)	
C15	0.3778 (5)	0.5963 (4)	0.1217 (3)	0.0957 (10)	
H15A	0.3317	0.5485	0.0482	0.115*	0.58 (4)
H15B	0.4855	0.6434	0.1157	0.115*	0.58 (4)
H15C	0.3093	0.6627	0.1404	0.115*	0.58 (4)
H15D	0.4193	0.6879	0.1547	0.115*	0.42 (4)
H15E	0.2655	0.5930	0.0871	0.115*	0.42 (4)
H15F	0.4417	0.5737	0.0625	0.115*	0.42 (4)
C16	0.4629 (3)	0.3749 (2)	0.2057 (2)	0.0634 (6)	
H16	0.5066	0.3588	0.1373	0.076*	
C17	0.4722 (3)	0.2827 (2)	0.2932 (2)	0.0591 (5)	
H17	0.5233	0.2050	0.2838	0.071*	
C18	0.4068 (2)	0.30246 (19)	0.39596 (18)	0.0500 (5)	
H18	0.4141	0.2391	0.4552	0.060*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0941 (5)	0.0763 (4)	0.0856 (5)	0.0268 (4)	0.0434 (4)	0.0205 (3)
C1	0.0660 (13)	0.0471 (11)	0.0538 (11)	0.0150 (9)	0.0065 (9)	0.0008 (9)

C2	0.0457 (10)	0.0383 (10)	0.0517 (10)	0.0097 (7)	0.0048 (8)	−0.0024 (8)
O1	0.0761 (10)	0.0348 (7)	0.0624 (9)	0.0128 (6)	0.0136 (7)	−0.0034 (6)
N1	0.0570 (9)	0.0306 (7)	0.0522 (9)	0.0080 (6)	0.0092 (7)	−0.0004 (6)
C3	0.0441 (10)	0.0387 (9)	0.0525 (11)	0.0120 (7)	0.0090 (8)	0.0004 (8)
C4	0.0528 (11)	0.0478 (10)	0.0551 (11)	0.0082 (9)	0.0089 (9)	−0.0041 (8)
C5	0.0609 (13)	0.0713 (14)	0.0532 (12)	0.0228 (11)	0.0086 (10)	−0.0025 (10)
C6	0.096 (2)	0.113 (2)	0.0581 (15)	0.0220 (17)	0.0037 (13)	−0.0182 (14)
C7	0.0863 (17)	0.0806 (17)	0.0607 (14)	0.0240 (14)	0.0256 (12)	0.0161 (12)
C8	0.0840 (17)	0.0607 (14)	0.0870 (18)	0.0042 (12)	0.0381 (14)	0.0144 (13)
C9	0.0550 (12)	0.0471 (11)	0.0674 (13)	0.0047 (9)	0.0160 (10)	−0.0012 (9)
Cl2	0.1420 (7)	0.0821 (5)	0.0695 (4)	0.0262 (4)	0.0490 (4)	0.0212 (3)
C10	0.0652 (13)	0.0455 (10)	0.0574 (12)	0.0059 (9)	0.0200 (10)	0.0012 (9)
C11	0.0464 (10)	0.0351 (9)	0.0555 (11)	0.0026 (7)	0.0089 (8)	0.0005 (8)
O2	0.0894 (11)	0.0347 (7)	0.0764 (10)	0.0123 (7)	0.0312 (8)	0.0091 (7)
N2	0.0530 (9)	0.0295 (7)	0.0540 (9)	0.0056 (6)	0.0144 (7)	−0.0001 (6)
C12	0.0413 (9)	0.0352 (9)	0.0500 (10)	−0.0007 (7)	0.0060 (8)	−0.0043 (7)
C13	0.0554 (11)	0.0431 (10)	0.0564 (11)	0.0104 (8)	0.0129 (9)	0.0025 (8)
C14	0.0697 (14)	0.0610 (13)	0.0536 (12)	0.0078 (10)	0.0169 (10)	0.0029 (10)
C15	0.136 (3)	0.099 (2)	0.0668 (17)	0.039 (2)	0.0418 (17)	0.0267 (15)
C16	0.0687 (14)	0.0658 (14)	0.0577 (13)	0.0052 (11)	0.0221 (10)	−0.0109 (10)
C17	0.0582 (12)	0.0476 (11)	0.0742 (14)	0.0101 (9)	0.0182 (10)	−0.0102 (10)
C18	0.0505 (11)	0.0399 (10)	0.0598 (12)	0.0072 (8)	0.0089 (9)	−0.0013 (8)

Geometric parameters (Å, º)

Cl1—C1	1.769 (2)	Cl2—C10	1.750 (2)
C1—C2	1.510 (3)	C10—C11	1.516 (3)
C1—H1A	0.9700	C10—H10A	0.9700
C1—H1B	0.9700	C10—H10B	0.9700
C2—O1	1.225 (2)	C11—O2	1.218 (2)
C2—N1	1.347 (2)	C11—N2	1.340 (2)
N1—C3	1.421 (3)	N2—C12	1.417 (3)
N1—H1	0.8600	N2—H2	0.8600
C3—C9	1.386 (3)	C12—C18	1.385 (3)
C3—C4	1.389 (3)	C12—C13	1.388 (3)
C4—C5	1.386 (3)	C13—C14	1.387 (3)
C4—H4	0.9300	C13—H13	0.9300
C5—C7	1.379 (4)	C14—C16	1.391 (3)
C5—C6	1.512 (4)	C14—C15	1.512 (3)
C6—H6A	0.9600	C15—H15A	0.9600
C6—H6B	0.9600	C15—H15B	0.9600
C6—H6C	0.9600	C15—H15C	0.9600
C6—H6D	0.9600	C15—H15D	0.9600
C6—H6E	0.9600	C15—H15E	0.9600
C6—H6F	0.9600	C15—H15F	0.9600
C7—C8	1.382 (4)	C16—C17	1.364 (3)
C7—H7	0.9300	C16—H16	0.9300
C8—C9	1.381 (3)	C17—C18	1.388 (3)

C8—H8	0.9300	C17—H17	0.9300
C9—H9	0.9300	C18—H18	0.9300
C2—C1—Cl1	109.99 (14)	C11—C10—Cl2	113.26 (15)
C2—C1—H1A	109.7	C11—C10—H10A	108.9
Cl1—C1—H1A	109.7	Cl2—C10—H10A	108.9
C2—C1—H1B	109.7	C11—C10—H10B	108.9
Cl1—C1—H1B	109.7	Cl2—C10—H10B	108.9
H1A—C1—H1B	108.2	H10A—C10—H10B	107.7
O1—C2—N1	124.31 (18)	O2—C11—N2	124.93 (19)
O1—C2—C1	121.44 (17)	O2—C11—C10	123.32 (18)
N1—C2—C1	114.25 (16)	N2—C11—C10	111.70 (16)
C2—N1—C3	126.86 (15)	C11—N2—C12	128.26 (16)
C2—N1—H1	116.6	C11—N2—H2	115.9
C3—N1—H1	116.6	C12—N2—H2	115.9
C9—C3—C4	120.1 (2)	C18—C12—C13	119.93 (18)
C9—C3—N1	122.24 (18)	C18—C12—N2	123.38 (17)
C4—C3—N1	117.60 (17)	C13—C12—N2	116.68 (17)
C5—C4—C3	121.0 (2)	C14—C13—C12	121.09 (19)
C5—C4—H4	119.5	C14—C13—H13	119.5
C3—C4—H4	119.5	C12—C13—H13	119.5
C7—C5—C4	118.3 (2)	C13—C14—C16	118.2 (2)
C7—C5—C6	121.8 (2)	C13—C14—C15	120.3 (2)
C4—C5—C6	119.9 (2)	C16—C14—C15	121.4 (2)
C5—C6—H6A	109.5	C14—C15—H15A	109.5
C5—C6—H6B	109.5	C14—C15—H15B	109.5
H6A—C6—H6B	109.5	H15A—C15—H15B	109.5
C5—C6—H6C	109.5	C14—C15—H15C	109.5
H6A—C6—H6C	109.5	H15A—C15—H15C	109.5
H6B—C6—H6C	109.5	H15B—C15—H15C	109.5
C5—C6—H6D	109.5	C14—C15—H15D	109.5
H6A—C6—H6D	141.1	H15A—C15—H15D	141.1
H6B—C6—H6D	56.3	H15B—C15—H15D	56.3
H6C—C6—H6D	56.3	H15C—C15—H15D	56.3
C5—C6—H6E	109.5	C14—C15—H15E	109.5
H6A—C6—H6E	56.3	H15A—C15—H15E	56.3
H6B—C6—H6E	141.1	H15B—C15—H15E	141.1
H6C—C6—H6E	56.3	H15C—C15—H15E	56.3
H6D—C6—H6E	109.5	H15D—C15—H15E	109.5
C5—C6—H6F	109.5	C14—C15—H15F	109.5
H6A—C6—H6F	56.3	H15A—C15—H15F	56.3
H6B—C6—H6F	56.3	H15B—C15—H15F	56.3
H6C—C6—H6F	141.1	H15C—C15—H15F	141.1
H6D—C6—H6F	109.5	H15D—C15—H15F	109.5
H6E—C6—H6F	109.5	H15E—C15—H15F	109.5
C5—C7—C8	120.9 (2)	C17—C16—C14	120.7 (2)
C5—C7—H7	119.6	C17—C16—H16	119.6
C8—C7—H7	119.6	C14—C16—H16	119.6

C9—C8—C7	120.8 (2)	C16—C17—C18	121.3 (2)
C9—C8—H8	119.6	C16—C17—H17	119.4
C7—C8—H8	119.6	C18—C17—H17	119.4
C8—C9—C3	118.8 (2)	C12—C18—C17	118.73 (19)
C8—C9—H9	120.6	C12—C18—H18	120.6
C3—C9—H9	120.6	C17—C18—H18	120.6
Cl1—C1—C2—O1	−63.8 (2)	Cl2—C10—C11—O2	16.0 (3)
Cl1—C1—C2—N1	116.98 (16)	Cl2—C10—C11—N2	−166.24 (14)
O1—C2—N1—C3	−0.3 (3)	O2—C11—N2—C12	1.1 (3)
C1—C2—N1—C3	178.88 (17)	C10—C11—N2—C12	−176.62 (18)
C2—N1—C3—C9	−35.4 (3)	C11—N2—C12—C18	−20.4 (3)
C2—N1—C3—C4	147.54 (19)	C11—N2—C12—C13	161.13 (18)
C9—C3—C4—C5	0.6 (3)	C18—C12—C13—C14	0.6 (3)
N1—C3—C4—C5	177.68 (18)	N2—C12—C13—C14	179.07 (18)
C3—C4—C5—C7	0.9 (3)	C12—C13—C14—C16	0.4 (3)
C3—C4—C5—C6	−179.0 (2)	C12—C13—C14—C15	179.5 (2)
C4—C5—C7—C8	−1.2 (4)	C13—C14—C16—C17	−1.0 (4)
C6—C5—C7—C8	178.6 (2)	C15—C14—C16—C17	179.9 (3)
C5—C7—C8—C9	0.2 (4)	C14—C16—C17—C18	0.7 (4)
C7—C8—C9—C3	1.3 (4)	C13—C12—C18—C17	−0.9 (3)
C4—C3—C9—C8	−1.7 (3)	N2—C12—C18—C17	−179.25 (17)
N1—C3—C9—C8	−178.6 (2)	C16—C17—C18—C12	0.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.04	2.891 (2)	171
N2—H2···O1	0.86	2.13	2.970 (2)	166

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