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2-Chloro-*N*-(3,4-dimethylphenyl)-acetamide

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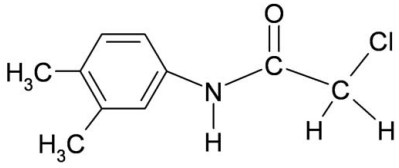
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.127; data-to-parameter ratio = 15.1.

The conformation of the C=O bond in the structure of the title compound, $C_{10}H_{12}ClNO$, is *anti* to the N—H bond and to the methylene H atoms in the side chain in both the independent molecules comprising the asymmetric unit. However, the conformation of the N—H bond is *syn* to the *meta*-methyl substituent in the aromatic ring of one of the molecules and *anti* in the other molecule. The two independent molecules are linked through intermolecular N—H···O hydrogen bonding into chains parallel to the *b* axis.

Related literature

For preparation of the compound, see: Shilpa & Gowda (2007). For related structures, see: Gowda *et al.* (2008*a*,*b*,*c*).



Experimental

Crystal data

$C_{10}H_{12}ClNO$ M_r = 197.66
Triclinic, $P\overline{1}$
a = 8.3672 (9) Å
b = 9.8076 (9) Å
c = 12.409 (1) Å
α = 95.415 (8)°
β = 96.492 (9)°
γ = 97.767 (9)°
V = 996.26 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 299 K
0.44 × 0.36 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.868, T_{max} = 0.936
10754 measured reflections
3634 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.127
S = 0.97
3634 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O2	0.86	2.05	2.8992 (16)	172
N2—H2*N*···O1^{i}	0.86	2.14	2.9802 (16)	166

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2441).

References

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supporting information

Acta Cryst. (2009). E**65**, o1022 [doi:10.1107/S1600536809013051]

2-Chloro-*N*-(3,4-dimethylphenyl)acetamide

B. Thimme Gowda, Sabine Foro, Hiromitsu Terao and Hartmut Fuess

S1. Comment

In the present work, as part of a study of the effect of ring and side chain substitutions on the crystal structures of aromatic amides (Gowda *et al.*, 2008a,b,c), the structure of 2-chloro-*N*-(3,4-dimethylphenyl)acetamide (I) has been determined. The asymmetric unit of the structure contains two molecules (Fig. 1). The conformation of the N—H bond is *syn* to the *meta*-methyl substituent in the aromatic ring of one of the molecules and *anti* in the other molecule. The conformation of the C=O bond in the structure is *anti* to the N—H bond and to the side chain methylene H-atoms in the side chain (Fig. 1), in both the independent molecules comprising the asymmetric unit, similar to that observed in in 2-chloro-*N*- (2,4-dimethylphenyl)acetamide (Gowda *et al.*, 2008*a*), in 2-chloro-*N*-(3,5-dichlorophenyl)acetamide (Gowda *et al.*, 2008*b*), and in 2-chloro-*N*-(3-methylphenyl)acetamide (Gowda *et al.*, 2008*c*). The two independent molecules in (I) are linked through intermolecular N—H···O hydrogen bonding (Fig.1) and the chains formed by H-bonding are parallel to the *b* axis (Table 1, Fig. 2).

S2. Experimental

Compound (I) was prepared according to the literature method (Shilpa & Gowda, 2007). Single crystals were obtained from the slow evaporation of an ethanolic solution of (I).

S3. Refinement

The H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.97 Å, N—H = 0.86 Å, and were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

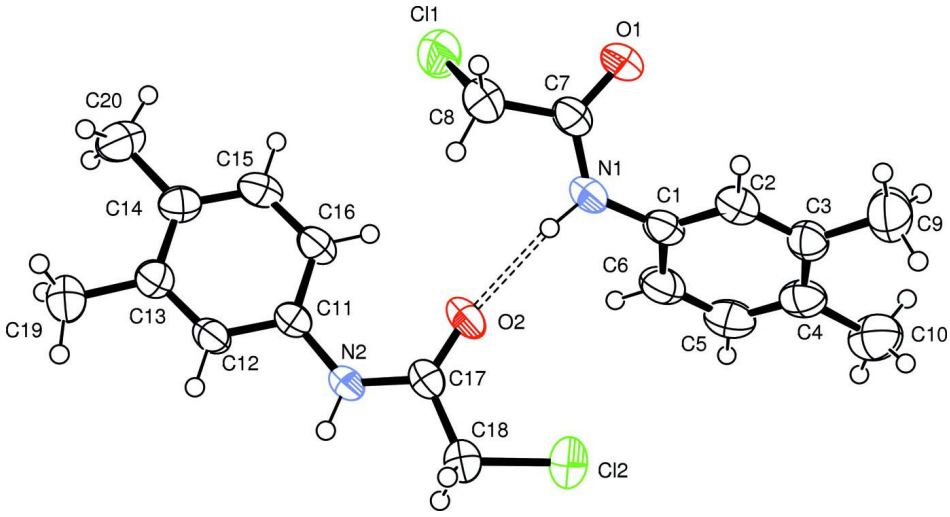

Figure 1

Molecular structure of (I), showing the atom labeling scheme and displacement ellipsoids drawn at the 50% probability level.

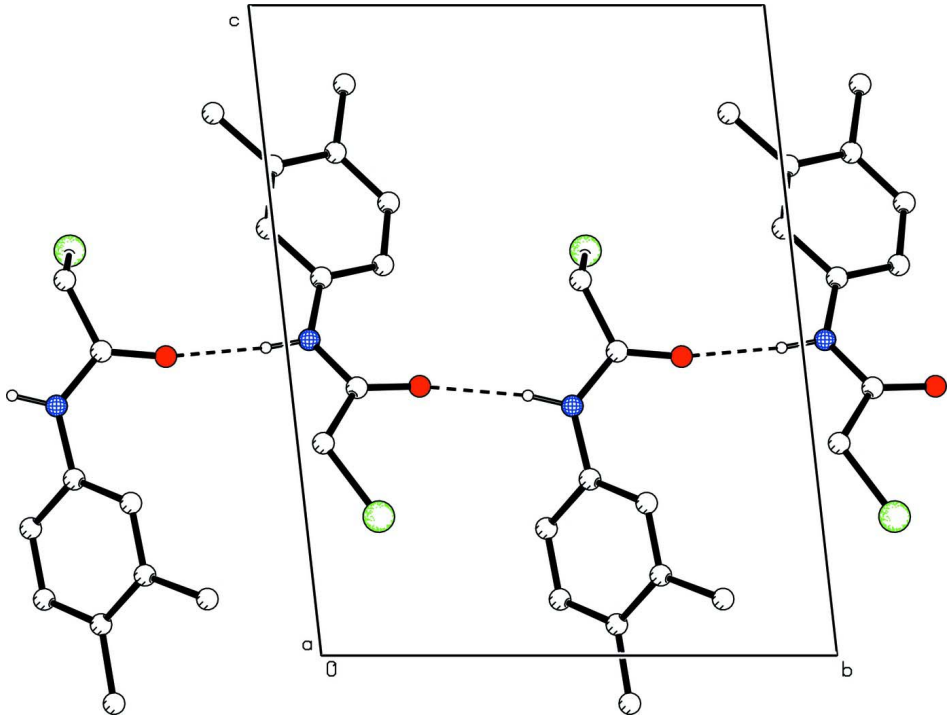

Figure 2

Molecular packing of (I) with hydrogen bonding shown as dashed lines.

2-Chloro-*N*-(3,4-dimethylphenyl)acetamide

Crystal data

$C_{10}H_{12}ClNO$
$M_r = 197.66$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.3672\ (9)$ Å
$b = 9.8076\ (9)$ Å

c = 12.409 (1) Å
α = 95.415 (8)°
β = 96.492 (9)°
γ = 97.767 (9)°
V = 996.26 (16) Å^3
Z = 4
F(000) = 416
D_x = 1.318 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4345 reflections
θ = 2.8–27.6°
μ = 0.34 mm^{-1}
T = 299 K
Rod, colourless
0.44 × 0.36 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Radiation source: fine-focus sealed tube
Graphite monochromator
Rotation method data acquisition using ω and φ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.868, T_{max} = 0.936

10754 measured reflections
3634 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.4°, θ_{min} = 2.8°
h = −10→10
k = −11→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.127
S = 0.97
3634 reflections
240 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.024 (4)

Special details

Experimental. Absorption correction: empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm, CrysAlis RED (Oxford Diffraction, 2007).

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}
Cl1	0.62739 (6)	0.60024 (5)	0.62240 (4)	0.0701 (2)
O1	0.83974 (16)	0.76355 (11)	0.45971 (10)	0.0569 (3)
N1	0.81699 (17)	0.54085 (13)	0.38380 (11)	0.0477 (3)
H1N	0.8113	0.4570	0.3998	0.057*
C1	0.81633 (19)	0.55916 (15)	0.27115 (14)	0.0447 (4)

C2	0.9174 (2)	0.66380 (16)	0.23435 (14)	0.0482 (4)
H2	0.9875	0.7272	0.2846	0.058*
C3	0.9155 (2)	0.67553 (17)	0.12342 (14)	0.0490 (4)
C4	0.8120 (2)	0.57967 (18)	0.04769 (14)	0.0542 (4)
C5	0.7129 (2)	0.47505 (18)	0.08636 (16)	0.0627 (5)
H5	0.6434	0.4105	0.0367	0.075*
C6	0.7148 (2)	0.46423 (17)	0.19551 (16)	0.0575 (5)
H6	0.6474	0.3926	0.2190	0.069*
C7	0.82545 (19)	0.63949 (16)	0.46785 (14)	0.0446 (4)
C8	0.8184 (2)	0.58415 (19)	0.57750 (14)	0.0546 (4)
H8A	0.9049	0.6356	0.6304	0.066*
H8B	0.8339	0.4876	0.5710	0.066*
C9	1.0278 (3)	0.7913 (2)	0.08682 (19)	0.0753 (6)
H9A	1.0907	0.8458	0.1495	0.090*
H9B	0.9646	0.8488	0.0466	0.090*
H9C	1.0995	0.7528	0.0411	0.090*
C10	0.8062 (3)	0.5877 (3)	−0.07390 (16)	0.0781 (6)
H10A	0.9126	0.5838	−0.0949	0.094*
H10B	0.7710	0.6731	−0.0913	0.094*
H10C	0.7314	0.5112	−0.1126	0.094*
Cl2	0.90424 (8)	0.14166 (5)	0.21372 (4)	0.0779 (2)
O2	0.78329 (17)	0.24929 (11)	0.41405 (11)	0.0628 (4)
N2	0.74319 (15)	0.04521 (12)	0.48565 (10)	0.0414 (3)
H2N	0.7539	−0.0406	0.4734	0.050*
C11	0.67313 (18)	0.08227 (14)	0.58097 (12)	0.0379 (3)
C12	0.66625 (19)	−0.01217 (15)	0.65716 (12)	0.0428 (4)
H12	0.7076	−0.0946	0.6435	0.051*
C13	0.5996 (2)	0.01258 (16)	0.75308 (13)	0.0458 (4)
C14	0.53726 (19)	0.13642 (16)	0.77369 (13)	0.0459 (4)
C15	0.5432 (2)	0.22884 (16)	0.69622 (14)	0.0503 (4)
H15	0.5011	0.3110	0.7092	0.060*
C16	0.60886 (19)	0.20418 (15)	0.60076 (14)	0.0466 (4)
H16	0.6102	0.2683	0.5501	0.056*
C17	0.79504 (19)	0.12730 (15)	0.41182 (13)	0.0425 (4)
C18	0.8760 (2)	0.05019 (18)	0.32656 (13)	0.0519 (4)
H18A	0.8097	−0.0386	0.3018	0.062*
H18B	0.9808	0.0326	0.3598	0.062*
C19	0.5979 (3)	−0.0922 (2)	0.83395 (16)	0.0698 (6)
H19A	0.6609	−0.0513	0.9016	0.084*
H19B	0.6439	−0.1707	0.8058	0.084*
H19C	0.4879	−0.1216	0.8462	0.084*
C20	0.4663 (2)	0.1688 (2)	0.87824 (15)	0.0639 (5)
H20A	0.5468	0.1673	0.9396	0.077*
H20B	0.3736	0.1008	0.8819	0.077*
H20C	0.4333	0.2589	0.8797	0.077*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0802 (4)	0.0660 (3)	0.0721 (3)	0.0167 (3)	0.0302 (3)	0.0161 (2)
O1	0.0811 (9)	0.0320 (6)	0.0606 (7)	0.0144 (5)	0.0136 (6)	0.0069 (5)
N1	0.0598 (9)	0.0290 (6)	0.0568 (8)	0.0085 (6)	0.0128 (7)	0.0085 (6)
C1	0.0469 (9)	0.0323 (7)	0.0568 (9)	0.0115 (7)	0.0090 (7)	0.0041 (7)
C2	0.0470 (9)	0.0380 (8)	0.0578 (10)	0.0046 (7)	0.0043 (8)	0.0017 (7)
C3	0.0500 (10)	0.0447 (9)	0.0559 (10)	0.0142 (7)	0.0101 (8)	0.0097 (7)
C4	0.0570 (10)	0.0513 (10)	0.0570 (10)	0.0243 (8)	0.0029 (8)	0.0020 (8)
C5	0.0653 (12)	0.0478 (10)	0.0682 (12)	0.0054 (9)	−0.0037 (10)	−0.0101 (8)
C6	0.0618 (11)	0.0374 (8)	0.0703 (12)	0.0011 (8)	0.0095 (9)	−0.0023 (8)
C7	0.0437 (9)	0.0356 (8)	0.0567 (9)	0.0099 (7)	0.0073 (7)	0.0093 (7)
C8	0.0596 (11)	0.0477 (9)	0.0584 (10)	0.0104 (8)	0.0066 (8)	0.0126 (8)
C9	0.0797 (14)	0.0735 (14)	0.0735 (13)	−0.0002 (11)	0.0189 (11)	0.0176 (11)
C10	0.0970 (17)	0.0832 (15)	0.0568 (12)	0.0346 (13)	−0.0021 (11)	0.0040 (10)
Cl2	0.1111 (5)	0.0687 (3)	0.0604 (3)	0.0094 (3)	0.0316 (3)	0.0223 (2)
O2	0.0880 (10)	0.0318 (6)	0.0763 (8)	0.0136 (6)	0.0275 (7)	0.0190 (6)
N2	0.0518 (8)	0.0259 (6)	0.0483 (7)	0.0061 (5)	0.0106 (6)	0.0073 (5)
C11	0.0379 (8)	0.0299 (7)	0.0447 (8)	0.0025 (6)	0.0036 (6)	0.0037 (6)
C12	0.0499 (9)	0.0299 (7)	0.0508 (9)	0.0097 (6)	0.0084 (7)	0.0073 (6)
C13	0.0516 (9)	0.0404 (8)	0.0446 (8)	0.0056 (7)	0.0048 (7)	0.0046 (7)
C14	0.0440 (9)	0.0428 (8)	0.0485 (9)	0.0040 (7)	0.0046 (7)	−0.0027 (7)
C15	0.0528 (10)	0.0358 (8)	0.0636 (10)	0.0134 (7)	0.0093 (8)	0.0003 (7)
C16	0.0519 (9)	0.0322 (7)	0.0581 (10)	0.0102 (7)	0.0080 (8)	0.0101 (7)
C17	0.0458 (9)	0.0334 (8)	0.0480 (9)	0.0021 (6)	0.0059 (7)	0.0091 (6)
C18	0.0618 (11)	0.0465 (9)	0.0510 (9)	0.0088 (8)	0.0151 (8)	0.0134 (7)
C19	0.0980 (16)	0.0619 (11)	0.0592 (11)	0.0223 (11)	0.0262 (11)	0.0215 (9)
C20	0.0684 (12)	0.0652 (12)	0.0567 (11)	0.0089 (10)	0.0157 (9)	−0.0078 (9)

Geometric parameters (Å, º)

Cl1—C8	1.7731 (19)	Cl2—C18	1.7539 (16)
O1—C7	1.2213 (18)	O2—C17	1.2117 (18)
N1—C7	1.343 (2)	N2—C17	1.3454 (19)
N1—C1	1.426 (2)	N2—C11	1.4171 (19)
N1—H1N	0.8600	N2—H2N	0.8600
C1—C6	1.382 (2)	C11—C12	1.385 (2)
C1—C2	1.385 (2)	C11—C16	1.388 (2)
C2—C3	1.391 (2)	C12—C13	1.385 (2)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.395 (2)	C13—C14	1.398 (2)
C3—C9	1.511 (3)	C13—C19	1.503 (2)
C4—C5	1.387 (3)	C14—C15	1.383 (2)
C4—C10	1.514 (3)	C14—C20	1.511 (2)
C5—C6	1.367 (3)	C15—C16	1.376 (2)
C5—H5	0.9300	C15—H15	0.9300
C6—H6	0.9300	C16—H16	0.9300

C7—C8	1.516 (2)	C17—C18	1.517 (2)
C8—H8A	0.9700	C18—H18A	0.9700
C8—H8B	0.9700	C18—H18B	0.9700
C9—H9A	0.9600	C19—H19A	0.9600
C9—H9B	0.9600	C19—H19B	0.9600
C9—H9C	0.9600	C19—H19C	0.9600
C10—H10A	0.9600	C20—H20A	0.9600
C10—H10B	0.9600	C20—H20B	0.9600
C10—H10C	0.9600	C20—H20C	0.9600
C7—N1—C1	127.45 (13)	C17—N2—C11	128.24 (12)
C7—N1—H1N	116.3	C17—N2—H2N	115.9
C1—N1—H1N	116.3	C11—N2—H2N	115.9
C6—C1—C2	118.88 (16)	C12—C11—C16	118.87 (14)
C6—C1—N1	118.09 (15)	C12—C11—N2	116.84 (13)
C2—C1—N1	122.98 (14)	C16—C11—N2	124.27 (13)
C1—C2—C3	120.99 (15)	C11—C12—C13	121.92 (14)
C1—C2—H2	119.5	C11—C12—H12	119.0
C3—C2—H2	119.5	C13—C12—H12	119.0
C2—C3—C4	119.72 (16)	C12—C13—C14	119.13 (15)
C2—C3—C9	119.26 (16)	C12—C13—C19	119.77 (15)
C4—C3—C9	121.02 (17)	C14—C13—C19	121.09 (16)
C5—C4—C3	118.29 (16)	C15—C14—C13	118.25 (15)
C5—C4—C10	120.04 (17)	C15—C14—C20	120.87 (16)
C3—C4—C10	121.68 (18)	C13—C14—C20	120.88 (16)
C6—C5—C4	121.78 (16)	C16—C15—C14	122.68 (15)
C6—C5—H5	119.1	C16—C15—H15	118.7
C4—C5—H5	119.1	C14—C15—H15	118.7
C5—C6—C1	120.34 (17)	C15—C16—C11	119.14 (14)
C5—C6—H6	119.8	C15—C16—H16	120.4
C1—C6—H6	119.8	C11—C16—H16	120.4
O1—C7—N1	124.51 (15)	O2—C17—N2	124.59 (15)
O1—C7—C8	121.48 (15)	O2—C17—C18	123.45 (14)
N1—C7—C8	114.00 (14)	N2—C17—C18	111.93 (13)
C7—C8—Cl1	109.74 (12)	C17—C18—Cl2	112.79 (12)
C7—C8—H8A	109.7	C17—C18—H18A	109.0
Cl1—C8—H8A	109.7	Cl2—C18—H18A	109.0
C7—C8—H8B	109.7	C17—C18—H18B	109.0
Cl1—C8—H8B	109.7	Cl2—C18—H18B	109.0
H8A—C8—H8B	108.2	H18A—C18—H18B	107.8
C3—C9—H9A	109.5	C13—C19—H19A	109.5
C3—C9—H9B	109.5	C13—C19—H19B	109.5
H9A—C9—H9B	109.5	H19A—C19—H19B	109.5
C3—C9—H9C	109.5	C13—C19—H19C	109.5
H9A—C9—H9C	109.5	H19A—C19—H19C	109.5
H9B—C9—H9C	109.5	H19B—C19—H19C	109.5
C4—C10—H10A	109.5	C14—C20—H20A	109.5
C4—C10—H10B	109.5	C14—C20—H20B	109.5

H10A—C10—H10B	109.5	H20A—C20—H20B	109.5
C4—C10—H10C	109.5	C14—C20—H20C	109.5
H10A—C10—H10C	109.5	H20A—C20—H20C	109.5
H10B—C10—H10C	109.5	H20B—C20—H20C	109.5
C7—N1—C1—C6	−140.52 (16)	C17—N2—C11—C12	−164.70 (14)
C7—N1—C1—C2	42.3 (2)	C17—N2—C11—C16	16.8 (2)
C6—C1—C2—C3	1.1 (2)	C16—C11—C12—C13	−1.1 (2)
N1—C1—C2—C3	178.30 (14)	N2—C11—C12—C13	−179.64 (14)
C1—C2—C3—C4	−0.8 (2)	C11—C12—C13—C14	0.1 (2)
C1—C2—C3—C9	180.00 (16)	C11—C12—C13—C19	−178.89 (16)
C2—C3—C4—C5	0.2 (2)	C12—C13—C14—C15	0.7 (2)
C9—C3—C4—C5	179.41 (17)	C19—C13—C14—C15	179.67 (16)
C2—C3—C4—C10	−179.69 (17)	C12—C13—C14—C20	−178.87 (15)
C9—C3—C4—C10	−0.5 (3)	C19—C13—C14—C20	0.1 (3)
C3—C4—C5—C6	0.0 (3)	C13—C14—C15—C16	−0.5 (3)
C10—C4—C5—C6	179.91 (18)	C20—C14—C15—C16	179.05 (16)
C4—C5—C6—C1	0.4 (3)	C14—C15—C16—C11	−0.5 (3)
C2—C1—C6—C5	−0.9 (3)	C12—C11—C16—C15	1.2 (2)
N1—C1—C6—C5	−178.21 (16)	N2—C11—C16—C15	179.71 (14)
C1—N1—C7—O1	−2.7 (3)	C11—N2—C17—O2	−3.0 (3)
C1—N1—C7—C8	178.29 (15)	C11—N2—C17—C18	175.03 (14)
O1—C7—C8—Cl1	73.33 (19)	O2—C17—C18—Cl2	−15.1 (2)
N1—C7—C8—Cl1	−107.59 (15)	N2—C17—C18—Cl2	166.82 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2	0.86	2.05	2.8992 (16)	172
N2—H2*N*···O1^{i}	0.86	2.14	2.9802 (16)	166

Symmetry code: (i) *x*, *y*−1, *z*.