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2,4-Bis(4-chlorophenyl)-3-azabicyclo-[3.3.1]nonan-9-one

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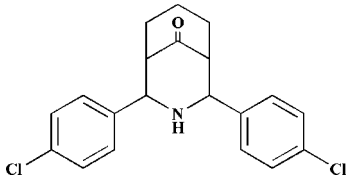
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.135; data-to-parameter ratio = 22.6.

In the molecular structure of the title compound, $C_{20}H_{19}Cl_2NO$, the molecule exists in a twin-chair conformation with equatorial dispositions of the 4-chlorophenyl groups on both sides of the secondary amino group; the dihedral angle between the aromatic ring planes is 31.33 (3)°. The crystal structure is stabilized by N—H···O interactions, leading to chains of molecules.

Related literature

For the biological activity of diterpenoid/norditerpenoid alkaloids, see: Hardick *et al.* (1996); Jeyaraman *et al.* (1981). For similiar structures, see: Parthiban *et al.* (2008*a*,*b*,*c*,*d*,*e*). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{20}H_{19}Cl_2NO$
M_r = 360.26
Monoclinic, $P2_1/n$
a = 16.2589 (4) Å
b = 6.8983 (2) Å
c = 18.1291 (5) Å
β = 116.149 (1)°
V = 1825.23 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 298 K
0.42 × 0.38 × 0.25 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.863, T_{max} = 0.915
15050 measured reflections
4997 independent reflections
3241 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.02
4997 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.85 (2)	2.31 (2)	3.1202 (18)	160.2 (18)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); 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: BQ2124).

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2,4-Bis(4-chlorophenyl)-3-azabicyclo[3.3.1]nonan-9-one

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S1. Comment

The widespread diterpenoid/norditerpenoid alkaloids posses the 3-azabicyclo [3.3.1]nonane pharmacophore, and as a consequence, the above alkaloids having broad spectrum of biological activities (Jeyaraman *et al.*, 1981; Hardick *et al.*, 1996). Hence, the synthesis and stereochemistry of 3-azabicyclononan-9-ones are more important in recent days (Parthiban *et al.*, 2008a,b,c,d,e). A study of torsion angles, asymmetry parameters and least-squares plane calculation shows that the piperidine ring adopts near ideal chair conformation with the deviation of ring atoms N1 and C8 from the C1/C2/C6/C7 plane by -0.642 (3)Å and 0.712 (3)Å, respectively, Q_T=0.607 (2)Å, q(2)=0.044 (2)Å and q(3)=-0.606 (2)Å, θ=175.8 (2)°. whereas the cyclohexane ring deviate from the ideal chair conformation; the cyclohexane atoms C4 and C8 deviate from the C2/C3/C5/C6 plane by -0.557 (2)Å and 0.710 (3)Å, respectively, Q_T=0.560 (2) Å, q(2)=0.117 (2)Å and, q(3)=-0.548 (2)Å, θ=167.9 (2)°. (Cremer & Pople, 1975). Hence, the title compound $C_{20}H_{19}Cl_2NO$, exists in double chair conformation with equatorial dispositions of the *para* chlorophenyl groups with the torsion angles of C8—C2—C1—C9 and C8—C6—C7—C15 are 177.88 (4)° and -179.01 (4)°, respectively. The aryl groups are oriented at an angle of 31.33 (3)° to each other.

S2. Experimental

In a warm solution of ammonium acetate (0.075 mol) in 50 ml of absolute ethanol, a mixture of cyclohexanone (0.05 mol) and *para* chlorobenzaldehyde (0.1 mol) was added and gently warmed with stirring on a hot plate till the yellow color was formed during the mixing of the reactants and cooled to room temperature. Then 50 ml of ether was added and allowed to stir over night at room temperature. Thus the obtained crude azabicyclic ketone was separated by filtration and washed with 1:5 ethanol-ether mixture till the solid became colorless. Recrystallization of the compound from ethanol gave X-ray diffraction quality crystals of 2,4-bis(4-chlorophenyl)-3-azabicyclo[3.3.1]nonan-9-one.

S3. Refinement

Nitrogen H atoms were located in a difference Fourier map and refined isotropically. Other hydrogen atoms were fixed geometrically and allowed to ride on the parent carbon atoms, with aromatic C—H =0.93Å, aliphatic C—H =0.98Å and methylene C—H=0.97Å. The displacement parameters were set for phenyl, methylene and aliphatic H atoms at U_{iso}(H)=1.2U_{eq}(C).

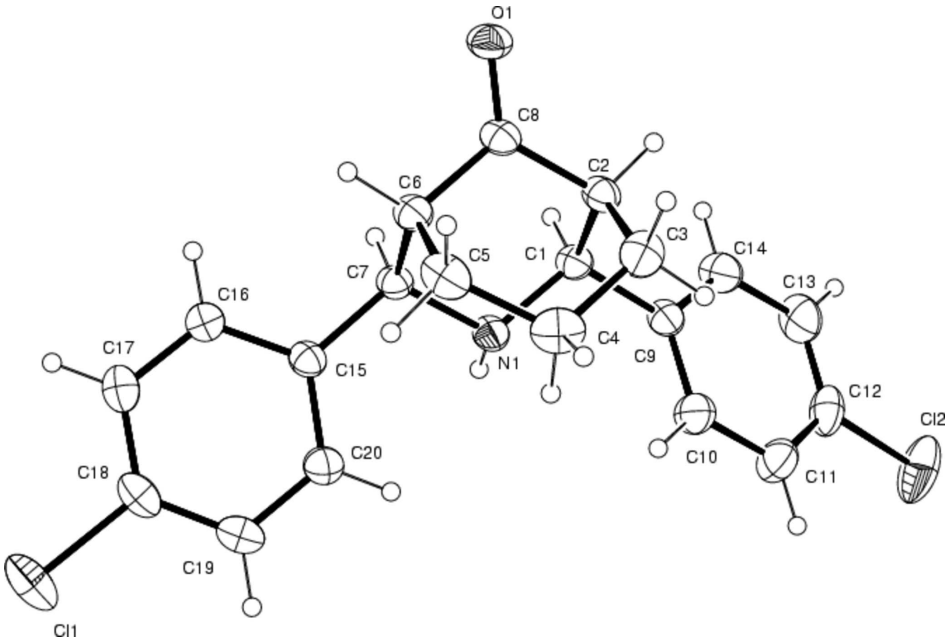

Figure 1

ORTEP of the molecule with atoms represented as 30% probability ellipsoids.

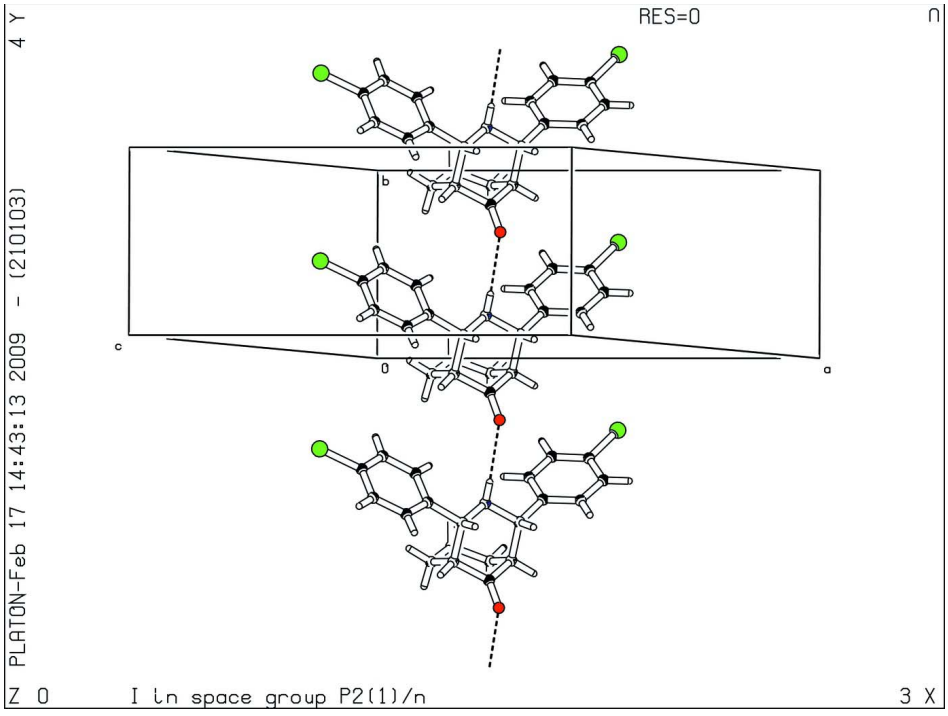

Figure 2

Packing of molecules via N-H..O bond.

2,4-Bis(4-chlorophenyl)-3-azabicyclo[3.3.1]nonan-9-one

Crystal data

$C_{20}H_{19}Cl_2NO$
M_r = 360.26
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 16.2589 (4) Å
b = 6.8983 (2) Å
c = 18.1291 (5) Å
β = 116.149 (1)°
V = 1825.23 (9) Å^3
Z = 4
F(000) = 752
D_x = 1.311 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4308 reflections
θ = 2.8–26.3°
μ = 0.36 mm^{-1}
T = 298 K
Rectangular, colourless
0.42 × 0.38 × 0.25 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.863, T_{max} = 0.915
15050 measured reflections
4997 independent reflections
3241 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 29.8°, θ_{min} = 2.3°
$h = -21 \rightarrow 20$
$k = -9 \rightarrow 9$
$l = -15 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.02
4997 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.4485P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.33305 (11)	0.1260 (2)	0.01759 (10)	0.0384 (3)
H1	0.3907	0.1019	0.0665	0.046*
C2	0.29289 (11)	−0.0738 (2)	−0.02171 (10)	0.0410 (4)
H2	0.3380	−0.1414	−0.0345	0.049*
C3	0.20110 (12)	−0.0678 (3)	−0.09929 (11)	0.0533 (4)
H3A	0.2079	0.0135	−0.1399	0.064*
H3B	0.1864	−0.1977	−0.1219	0.064*
C4	0.12129 (12)	0.0082 (3)	−0.08496 (12)	0.0581 (5)
H4A	0.1268	0.1478	−0.0779	0.070*
H4B	0.0643	−0.0190	−0.1330	0.070*
C5	0.11811 (12)	−0.0827 (3)	−0.00979 (12)	0.0534 (5)
H5A	0.0944	−0.2136	−0.0235	0.064*
H5B	0.0756	−0.0096	0.0037	0.064*
C6	0.21147 (11)	−0.0905 (2)	0.06658 (11)	0.0418 (4)
H6	0.2052	−0.1688	0.1090	0.050*
C7	0.25223 (11)	0.1109 (2)	0.10384 (10)	0.0375 (3)
H7	0.3106	0.0893	0.1524	0.045*
C8	0.27891 (11)	−0.1870 (2)	0.04285 (10)	0.0390 (4)
C9	0.35398 (11)	0.2533 (2)	−0.03978 (10)	0.0414 (4)
C10	0.29057 (13)	0.3777 (3)	−0.09592 (12)	0.0544 (5)
H10	0.2316	0.3836	−0.1000	0.065*
C11	0.31400 (15)	0.4943 (3)	−0.14645 (12)	0.0615 (5)
H11	0.2710	0.5776	−0.1841	0.074*
C12	0.40091 (16)	0.4852 (3)	−0.14022 (12)	0.0584 (5)
C13	0.46439 (15)	0.3618 (3)	−0.08633 (14)	0.0654 (6)
H13	0.5228	0.3545	−0.0835	0.078*
C14	0.44093 (13)	0.2474 (3)	−0.03588 (13)	0.0555 (5)
H14	0.4845	0.1646	0.0015	0.067*
C15	0.18866 (11)	0.2164 (2)	0.13081 (10)	0.0385 (3)
C16	0.17785 (12)	0.1464 (3)	0.19803 (11)	0.0473 (4)
H16	0.2125	0.0407	0.2271	0.057*
C17	0.11692 (13)	0.2301 (3)	0.22247 (11)	0.0528 (4)
H17	0.1097	0.1804	0.2670	0.063*
C18	0.06701 (12)	0.3877 (3)	0.18023 (12)	0.0509 (4)
C19	0.07748 (13)	0.4646 (3)	0.11480 (12)	0.0540 (5)
H19	0.0446	0.5740	0.0877	0.065*
C20	0.13769 (12)	0.3765 (2)	0.08997 (11)	0.0471 (4)
H20	0.1440	0.4259	0.0450	0.057*
Cl1	−0.01108 (4)	0.49239 (10)	0.21027 (4)	0.0838 (2)
Cl2	0.43337 (5)	0.64178 (11)	−0.19813 (4)	0.0956 (3)
N1	0.27045 (9)	0.2229 (2)	0.04419 (9)	0.0401 (3)
O1	0.31840 (9)	−0.33704 (16)	0.07301 (8)	0.0515 (3)
H1A	0.2917 (13)	0.334 (3)	0.0645 (12)	0.058 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0379 (8)	0.0331 (8)	0.0479 (9)	−0.0024 (6)	0.0223 (7)	0.0015 (7)
C2	0.0440 (9)	0.0329 (8)	0.0532 (9)	−0.0007 (7)	0.0278 (8)	−0.0020 (7)
C3	0.0591 (11)	0.0489 (10)	0.0498 (10)	−0.0103 (9)	0.0221 (9)	−0.0051 (8)
C4	0.0413 (10)	0.0552 (12)	0.0634 (12)	−0.0046 (8)	0.0100 (9)	−0.0021 (10)
C5	0.0407 (9)	0.0473 (10)	0.0750 (13)	−0.0100 (8)	0.0279 (9)	−0.0112 (9)
C6	0.0462 (9)	0.0304 (8)	0.0578 (10)	−0.0030 (7)	0.0312 (8)	0.0018 (7)
C7	0.0387 (8)	0.0317 (7)	0.0458 (9)	0.0003 (6)	0.0218 (7)	0.0016 (7)
C8	0.0401 (8)	0.0273 (7)	0.0514 (9)	−0.0059 (6)	0.0219 (7)	−0.0053 (7)
C9	0.0470 (9)	0.0327 (8)	0.0530 (9)	−0.0049 (7)	0.0298 (8)	−0.0023 (7)
C10	0.0526 (11)	0.0557 (11)	0.0635 (11)	0.0042 (9)	0.0334 (9)	0.0110 (9)
C11	0.0770 (14)	0.0560 (12)	0.0556 (11)	0.0002 (10)	0.0331 (11)	0.0112 (9)
C12	0.0821 (14)	0.0544 (11)	0.0527 (10)	−0.0244 (10)	0.0424 (10)	−0.0081 (9)
C13	0.0637 (13)	0.0668 (13)	0.0862 (15)	−0.0121 (11)	0.0517 (12)	0.0008 (12)
C14	0.0514 (11)	0.0483 (10)	0.0781 (13)	−0.0017 (8)	0.0387 (10)	0.0053 (9)
C15	0.0397 (8)	0.0334 (8)	0.0445 (8)	−0.0023 (6)	0.0205 (7)	−0.0035 (7)
C16	0.0531 (10)	0.0452 (10)	0.0471 (9)	0.0052 (8)	0.0254 (8)	0.0035 (8)
C17	0.0584 (11)	0.0601 (12)	0.0475 (10)	−0.0022 (9)	0.0305 (9)	−0.0062 (9)
C18	0.0442 (10)	0.0534 (11)	0.0576 (11)	−0.0012 (8)	0.0249 (9)	−0.0186 (9)
C19	0.0515 (11)	0.0435 (10)	0.0654 (12)	0.0096 (8)	0.0243 (9)	−0.0027 (9)
C20	0.0534 (10)	0.0394 (9)	0.0528 (10)	0.0025 (8)	0.0274 (8)	0.0022 (8)
Cl1	0.0721 (4)	0.0962 (5)	0.0986 (5)	0.0135 (3)	0.0519 (3)	−0.0262 (4)
Cl2	0.1246 (6)	0.1079 (5)	0.0667 (4)	−0.0502 (4)	0.0535 (4)	0.0061 (3)
N1	0.0490 (8)	0.0274 (6)	0.0524 (8)	−0.0046 (6)	0.0302 (7)	−0.0020 (6)
O1	0.0613 (8)	0.0313 (6)	0.0686 (8)	0.0042 (5)	0.0347 (7)	0.0037 (6)

Geometric parameters (Å, º)

C1—N1	1.466 (2)	C9—C10	1.382 (3)
C1—C9	1.511 (2)	C9—C14	1.385 (2)
C1—C2	1.557 (2)	C10—C11	1.393 (3)
C1—H1	0.9800	C10—H10	0.9300
C2—C8	1.505 (2)	C11—C12	1.368 (3)
C2—C3	1.535 (2)	C11—H11	0.9300
C2—H2	0.9800	C12—C13	1.363 (3)
C3—C4	1.524 (3)	C12—Cl2	1.7422 (18)
C3—H3A	0.9700	C13—C14	1.383 (3)
C3—H3B	0.9700	C13—H13	0.9300
C4—C5	1.522 (3)	C14—H14	0.9300
C4—H4A	0.9700	C15—C20	1.383 (2)
C4—H4B	0.9700	C15—C16	1.392 (2)
C5—C6	1.540 (3)	C16—C17	1.378 (2)
C5—H5A	0.9700	C16—H16	0.9300
C5—H5B	0.9700	C17—C18	1.371 (3)
C6—C8	1.499 (2)	C17—H17	0.9300
C6—C7	1.559 (2)	C18—C19	1.377 (3)

C6—H6	0.9800	C18—Cl1	1.7433 (17)
C7—N1	1.462 (2)	C19—C20	1.385 (2)
C7—C15	1.511 (2)	C19—H19	0.9300
C7—H7	0.9800	C20—H20	0.9300
C8—O1	1.2137 (19)	N1—H1A	0.85 (2)

N1—C1—C9	111.16 (13)	O1—C8—C6	123.91 (15)
N1—C1—C2	110.05 (12)	O1—C8—C2	124.16 (15)
C9—C1—C2	112.08 (13)	C6—C8—C2	111.92 (13)
N1—C1—H1	107.8	C10—C9—C14	118.01 (16)
C9—C1—H1	107.8	C10—C9—C1	123.14 (15)
C2—C1—H1	107.8	C14—C9—C1	118.85 (16)
C8—C2—C3	107.89 (13)	C9—C10—C11	120.76 (18)
C8—C2—C1	106.25 (13)	C9—C10—H10	119.6
C3—C2—C1	115.97 (14)	C11—C10—H10	119.6
C8—C2—H2	108.8	C12—C11—C10	119.42 (19)
C3—C2—H2	108.8	C12—C11—H11	120.3
C1—C2—H2	108.8	C10—C11—H11	120.3
C4—C3—C2	114.21 (15)	C13—C12—C11	121.07 (17)
C4—C3—H3A	108.7	C13—C12—Cl2	118.99 (16)
C2—C3—H3A	108.7	C11—C12—Cl2	119.86 (18)
C4—C3—H3B	108.7	C12—C13—C14	119.24 (19)
C2—C3—H3B	108.7	C12—C13—H13	120.4
H3A—C3—H3B	107.6	C14—C13—H13	120.4
C5—C4—C3	112.21 (16)	C13—C14—C9	121.49 (19)
C5—C4—H4A	109.2	C13—C14—H14	119.3
C3—C4—H4A	109.2	C9—C14—H14	119.3
C5—C4—H4B	109.2	C20—C15—C16	117.94 (15)
C3—C4—H4B	109.2	C20—C15—C7	123.06 (14)
H4A—C4—H4B	107.9	C16—C15—C7	118.96 (14)
C4—C5—C6	114.24 (14)	C17—C16—C15	121.48 (17)
C4—C5—H5A	108.7	C17—C16—H16	119.3
C6—C5—H5A	108.7	C15—C16—H16	119.3
C4—C5—H5B	108.7	C18—C17—C16	119.03 (17)
C6—C5—H5B	108.7	C18—C17—H17	120.5
H5A—C5—H5B	107.6	C16—C17—H17	120.5
C8—C6—C5	108.27 (14)	C17—C18—C19	121.29 (16)
C8—C6—C7	107.15 (12)	C17—C18—Cl1	119.16 (15)
C5—C6—C7	114.88 (14)	C19—C18—Cl1	119.55 (15)
C8—C6—H6	108.8	C18—C19—C20	118.97 (17)
C5—C6—H6	108.8	C18—C19—H19	120.5
C7—C6—H6	108.8	C20—C19—H19	120.5
N1—C7—C15	112.03 (12)	C15—C20—C19	121.25 (17)
N1—C7—C6	109.68 (13)	C15—C20—H20	119.4
C15—C7—C6	110.42 (12)	C19—C20—H20	119.4
N1—C7—H7	108.2	C7—N1—C1	113.48 (12)
C15—C7—H7	108.2	C7—N1—H1A	109.2 (14)
C6—C7—H7	108.2	C1—N1—H1A	110.1 (13)

N1—C1—C2—C8	−57.87 (16)	C1—C9—C10—C11	178.93 (17)
C9—C1—C2—C8	177.89 (13)	C9—C10—C11—C12	0.0 (3)
N1—C1—C2—C3	61.99 (18)	C10—C11—C12—C13	1.1 (3)
C9—C1—C2—C3	−62.25 (18)	C10—C11—C12—Cl2	−175.72 (16)
C8—C2—C3—C4	53.9 (2)	C11—C12—C13—C14	−1.5 (3)
C1—C2—C3—C4	−65.1 (2)	Cl2—C12—C13—C14	175.27 (16)
C2—C3—C4—C5	−46.3 (2)	C12—C13—C14—C9	1.0 (3)
C3—C4—C5—C6	45.7 (2)	C10—C9—C14—C13	0.0 (3)
C4—C5—C6—C8	−53.0 (2)	C1—C9—C14—C13	−179.45 (18)
C4—C5—C6—C7	66.6 (2)	N1—C7—C15—C20	14.1 (2)
C8—C6—C7—N1	57.05 (17)	C6—C7—C15—C20	−108.49 (17)
C5—C6—C7—N1	−63.26 (17)	N1—C7—C15—C16	−168.34 (15)
C8—C6—C7—C15	−179.02 (13)	C6—C7—C15—C16	69.09 (19)
C5—C6—C7—C15	60.67 (18)	C20—C15—C16—C17	1.5 (3)
C5—C6—C8—O1	−118.50 (18)	C7—C15—C16—C17	−176.24 (16)
C7—C6—C8—O1	117.07 (17)	C15—C16—C17—C18	−1.0 (3)
C5—C6—C8—C2	62.45 (17)	C16—C17—C18—C19	−0.8 (3)
C7—C6—C8—C2	−61.98 (17)	C16—C17—C18—Cl1	179.30 (14)
C3—C2—C8—O1	118.08 (18)	C17—C18—C19—C20	2.0 (3)
C1—C2—C8—O1	−116.94 (17)	Cl1—C18—C19—C20	−178.05 (14)
C3—C2—C8—C6	−62.87 (17)	C16—C15—C20—C19	−0.2 (3)
C1—C2—C8—C6	62.11 (17)	C7—C15—C20—C19	177.44 (16)
N1—C1—C9—C10	−35.0 (2)	C18—C19—C20—C15	−1.5 (3)
C2—C1—C9—C10	88.57 (19)	C15—C7—N1—C1	179.14 (13)
N1—C1—C9—C14	144.36 (16)	C6—C7—N1—C1	−57.87 (17)
C2—C1—C9—C14	−92.02 (19)	C9—C1—N1—C7	−176.47 (13)
C14—C9—C10—C11	−0.5 (3)	C2—C1—N1—C7	58.76 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.85 (2)	2.31 (2)	3.1202 (18)	160.2 (18)

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