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

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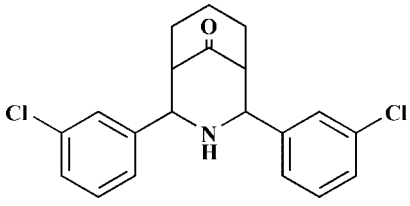
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.084; data-to-parameter ratio = 19.4.

In the molecular structure of the title compound, $C_{20}H_{19}Cl_2NO$, the bicyclic system adopts a twin-chair conformation with equatorial orientations of both substituents. The dihedral angle between the aromatic rings is 43.60 (2)° with respect to each other. The crystal structure is stabilized by weak N—H···O and strong C—H···O interactions.

Related literature

For the biological significance, synthesis and stereochemistry of 3-azabicyclononan-9-ones, see: Jeyaraman & Avila (1981). For similiar structures, see: Parthiban *et al.* (2008*a*,*b*,*c*,*d*,*e*). For puckering parameters, see: Web & Becker (1967); Cremer & Pople (1975).



Experimental

Crystal data

$C_{20}H_{19}Cl_2NO$
M_r = 360.26
Orthorhombic, $P2_12_12_1$
a = 6.9950 (14) Å
b = 12.180 (2) Å
c = 20.770 (4) Å
V = 1769.6 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 298 K
0.31 × 0.25 × 0.22 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.875, T_{max} = 0.922
23614 measured reflections
4284 independent reflections
2762 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.084
S = 1.01
4284 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 1756 Friedel pairs
Flack parameter: −0.05 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.83 (2)	2.35 (2)	3.129 (3)	155.4 (18)
C7—H7···O1^{ii}	0.98	2.44	3.296 (2)	146

Symmetry codes: (i) $x+1, y, z$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+2$.

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: GW2060).

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Acta Cryst. (2009). E**65**, o840 [doi:10.1107/S1600536809009945]

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

P. Parthiban, V. Ramkumar, H. D. Santan, Jong Tae Kim and Yeon Tae Jeong

S1. Comment

Due to their biological significance (Jeyaraman & Avila, 1981), the synthesis and stereochemistry of 3-azabicyclo-nonan-9-ones are more important in current affairs (Parthiban *et al.*, 2008*a*,*b*,*c*,*d*,*e*). The title compound C_{20} H_{19} Cl_2 N O, exists in twin-chair conformation with equatorial orientations of the *meta* chlorophenyl groups on both sides of the secondary amino group with the torsion angles of C8—C2—C1—C9 and C8—C6—C7—C15 are -177.78 (4)and 177.42 (3)°, respectively. 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 -0.669 (2) and 0.704 (3) Å, respectively, Q_T = 0.617 (2) Å, q(2)=0.021 (2) and q(3)=0.617 (2) Å, θ = 2.71 (19)°. (Cremer & Pople, 1975; Web & Becker, 1967) 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 -0.545 (4) and 0.714 (3)°, respectively, Q_T = 0.562 (2) Å, q(2)=0.128 (2) and q(3)=0.549 (2) Å, θ = 12.7 (2)°. (Cremer & Pople, 1975). The aryl groups are oriented at an angle of 43.60 (2)° to each other.

The crystal structure is stabilized by weak N—H···O (3.129 (3)Å and strong C—H···O interactions [C1—H···O1 (3.46 (3)Å and C7—H···O1 3.296 (2) Å]. Interestingly,the same acceptor O1 is involved in trifurcated hydrogen bond with N1,C1 and C7 where the Oxygen atoms is at the apex forming a tripyramidal.

S2. Experimental

A mixture of cyclohexanone (0.05 mol) and *meta* chlorobenzaldehyde (0.1 mol) was added to a warm solution of ammonium acetate (0.075 mol) in 50 ml of absolute ethanol. The mixture was gently warmed 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. At the end, the crude azabicyclic ketone was separated by filtration and washed with 1:5 ethanol-ether mixture till the solid became colourless. Recrystallization of the compound from ethanol gave X-ray diffraction quality crystals of 2,4-bis(3-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 =0.93 Å, aliphatic C—H = 0.98Å and methylen C—H = 0.97 Å. The displacement parameters were set for phenyl,methylen and aliphatic H atoms at U_{iso}(H) = 1.2U_{eq}(C).

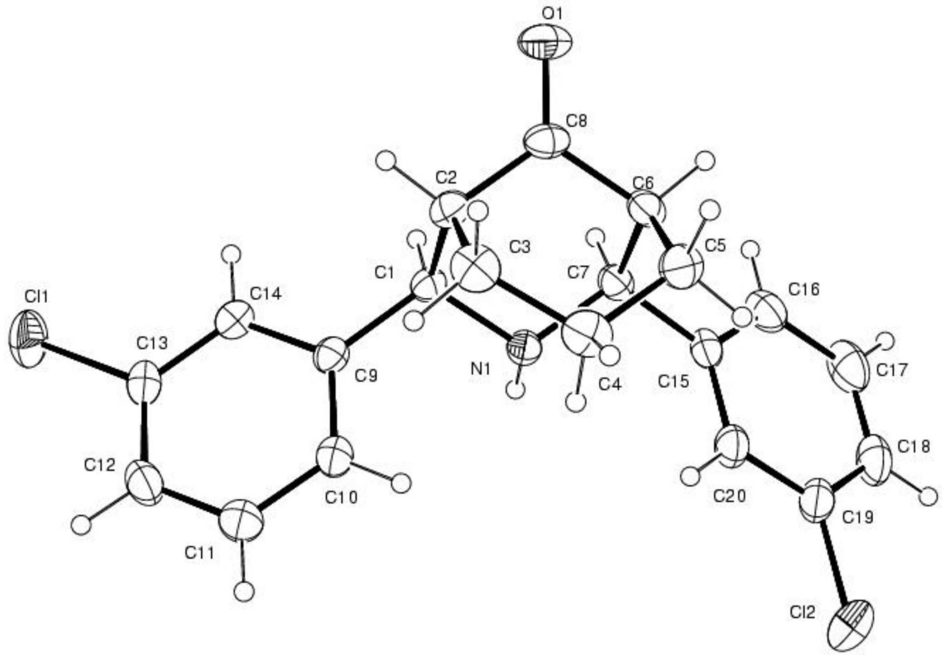

Figure 1

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

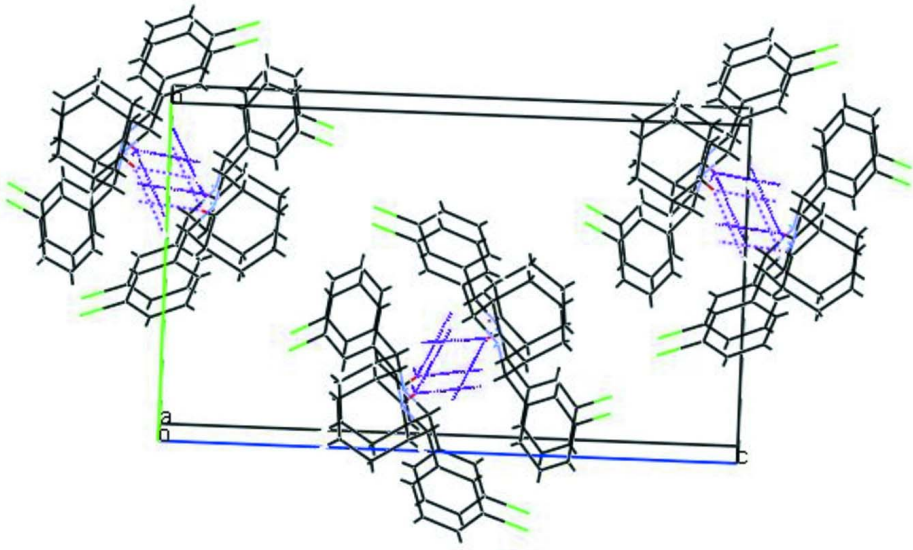

Figure 2

Packing diagram of molecules showing the N—H···O and C—H···O interactions.

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

Crystal data

$C_{20}H_{19}Cl_2NO$
M_r = 360.26
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 6.9950 (14) Å
b = 12.180 (2) Å
c = 20.770 (4) Å
V = 1769.6 (6) Å^3
Z = 4
F(000) = 752

D_x = 1.352 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5421 reflections
θ = 2.6–22.5°
μ = 0.37 mm^{-1}
T = 298 K
Block, colourless
0.31 × 0.25 × 0.22 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.875, T_{max} = 0.922
23614 measured reflections
4284 independent reflections
2762 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 28.3°, θ_{min} = 2.6°
h = −8→9
k = −16→16
l = −27→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.084
S = 1.01
4284 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
$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 0.181P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 1756 Friedel pairs
Absolute structure parameter: −0.05 (5)

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}
C1	0.1155 (3)	0.91094 (15)	0.96470 (9)	0.0351 (5)
H1	0.0839	0.8690	1.0035	0.042*
C2	−0.0754 (3)	0.94712 (17)	0.93253 (10)	0.0425 (5)
H2	−0.1483	0.9910	0.9635	0.051*
C3	−0.0574 (3)	1.01301 (18)	0.86920 (11)	0.0522 (6)
H3A	−0.1829	1.0398	0.8571	0.063*

H3B	0.0236	1.0763	0.8768	0.063*
C4	0.0248 (4)	0.94740 (18)	0.81344 (10)	0.0517 (6)
H4A	0.0035	0.9874	0.7737	0.062*
H4B	0.1617	0.9400	0.8193	0.062*
C5	−0.0633 (3)	0.83391 (19)	0.80751 (10)	0.0493 (6)
H5A	0.0141	0.7906	0.7782	0.059*
H5B	−0.1894	0.8411	0.7886	0.059*
C6	−0.0815 (3)	0.77124 (16)	0.87165 (10)	0.0405 (5)
H6	−0.1583	0.7050	0.8646	0.049*
C7	0.1088 (3)	0.73829 (16)	0.90524 (9)	0.0373 (5)
H7	0.0767	0.7017	0.9459	0.045*
C8	−0.1852 (3)	0.84501 (17)	0.91799 (9)	0.0417 (5)
C9	0.2390 (3)	1.00628 (15)	0.98456 (9)	0.0353 (5)
C10	0.3661 (3)	1.05578 (17)	0.94271 (10)	0.0485 (6)
H10	0.3780	1.0292	0.9009	0.058*
C11	0.4763 (4)	1.14476 (18)	0.96219 (12)	0.0589 (7)
H11	0.5609	1.1773	0.9334	0.071*
C12	0.4608 (3)	1.18510 (18)	1.02405 (11)	0.0514 (6)
H12	0.5330	1.2452	1.0372	0.062*
C13	0.3367 (3)	1.13481 (15)	1.06568 (10)	0.0430 (5)
C14	0.2249 (3)	1.04678 (16)	1.04695 (9)	0.0399 (5)
H14	0.1404	1.0148	1.0760	0.048*
C15	0.2255 (3)	0.65933 (15)	0.86531 (10)	0.0388 (5)
C16	0.2048 (3)	0.54727 (17)	0.87560 (12)	0.0543 (6)
H16	0.1230	0.5222	0.9077	0.065*
C17	0.3056 (4)	0.47232 (18)	0.83825 (15)	0.0679 (8)
H17	0.2895	0.3975	0.8453	0.081*
C18	0.4283 (4)	0.5073 (2)	0.79115 (13)	0.0619 (7)
H18	0.4961	0.4570	0.7664	0.074*
C19	0.4494 (3)	0.61781 (19)	0.78124 (12)	0.0514 (6)
C20	0.3510 (3)	0.69381 (17)	0.81787 (10)	0.0457 (5)
H20	0.3692	0.7684	0.8106	0.055*
Cl1	0.32230 (11)	1.18133 (5)	1.14500 (3)	0.0681 (2)
Cl2	0.60281 (11)	0.66335 (6)	0.72080 (3)	0.0794 (2)
N1	0.2172 (3)	0.83753 (13)	0.92051 (8)	0.0358 (4)
O1	−0.3405 (2)	0.82264 (14)	0.94107 (7)	0.0583 (4)
H1A	0.324 (3)	0.8184 (15)	0.9342 (9)	0.033 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0369 (12)	0.0377 (11)	0.0307 (9)	−0.0016 (9)	0.0059 (9)	−0.0005 (9)
C2	0.0360 (12)	0.0472 (12)	0.0443 (12)	0.0048 (10)	0.0048 (10)	−0.0061 (10)
C3	0.0502 (15)	0.0476 (13)	0.0587 (15)	0.0068 (11)	−0.0079 (12)	0.0076 (11)
C4	0.0549 (14)	0.0579 (14)	0.0421 (12)	−0.0040 (12)	−0.0058 (11)	0.0153 (11)
C5	0.0462 (14)	0.0647 (14)	0.0370 (11)	0.0005 (12)	−0.0065 (10)	0.0008 (11)
C6	0.0358 (12)	0.0435 (12)	0.0421 (12)	−0.0079 (10)	−0.0046 (10)	−0.0016 (9)
C7	0.0386 (12)	0.0371 (11)	0.0363 (11)	−0.0059 (10)	−0.0013 (9)	0.0008 (9)

C8	0.0307 (12)	0.0577 (13)	0.0366 (11)	0.0013 (11)	−0.0007 (10)	0.0090 (10)
C9	0.0347 (11)	0.0353 (11)	0.0359 (11)	0.0048 (9)	0.0008 (9)	−0.0016 (9)
C10	0.0553 (14)	0.0469 (12)	0.0433 (12)	−0.0088 (12)	0.0088 (11)	−0.0102 (10)
C11	0.0656 (16)	0.0530 (15)	0.0580 (14)	−0.0152 (13)	0.0154 (13)	−0.0035 (12)
C12	0.0536 (15)	0.0388 (12)	0.0619 (15)	−0.0075 (12)	−0.0048 (12)	−0.0081 (11)
C13	0.0500 (13)	0.0381 (11)	0.0409 (11)	0.0058 (10)	−0.0065 (11)	−0.0082 (9)
C14	0.0406 (12)	0.0422 (11)	0.0368 (11)	0.0054 (10)	0.0017 (9)	0.0006 (9)
C15	0.0396 (12)	0.0355 (11)	0.0412 (11)	−0.0008 (9)	−0.0085 (10)	−0.0074 (9)
C16	0.0499 (15)	0.0423 (13)	0.0708 (16)	−0.0074 (12)	−0.0046 (12)	−0.0040 (11)
C17	0.0720 (19)	0.0362 (13)	0.096 (2)	0.0028 (13)	−0.0140 (17)	−0.0134 (13)
C18	0.0565 (16)	0.0550 (16)	0.0743 (18)	0.0137 (13)	−0.0127 (15)	−0.0296 (14)
C19	0.0460 (14)	0.0588 (15)	0.0494 (13)	0.0060 (11)	−0.0049 (11)	−0.0193 (11)
C20	0.0507 (13)	0.0386 (11)	0.0477 (12)	0.0012 (11)	−0.0006 (11)	−0.0109 (10)
Cl1	0.0959 (5)	0.0649 (4)	0.0435 (3)	−0.0048 (4)	−0.0084 (3)	−0.0171 (3)
Cl2	0.0814 (5)	0.0891 (5)	0.0675 (4)	0.0069 (4)	0.0235 (4)	−0.0261 (4)
N1	0.0305 (10)	0.0393 (9)	0.0376 (9)	0.0018 (9)	−0.0019 (8)	−0.0052 (8)
O1	0.0363 (9)	0.0793 (11)	0.0593 (10)	−0.0063 (9)	0.0087 (8)	0.0071 (9)

Geometric parameters (Å, º)

C1—N1	1.465 (2)	C9—C10	1.382 (3)
C1—C9	1.505 (3)	C9—C14	1.390 (3)
C1—C2	1.557 (3)	C10—C11	1.390 (3)
C1—H1	0.9800	C10—H10	0.9300
C2—C8	1.493 (3)	C11—C12	1.380 (3)
C2—C3	1.546 (3)	C11—H11	0.9300
C2—H2	0.9800	C12—C13	1.369 (3)
C3—C4	1.520 (3)	C12—H12	0.9300
C3—H3A	0.9700	C13—C14	1.383 (3)
C3—H3B	0.9700	C13—Cl1	1.745 (2)
C4—C5	1.518 (3)	C14—H14	0.9300
C4—H4A	0.9700	C15—C16	1.389 (3)
C4—H4B	0.9700	C15—C20	1.385 (3)
C5—C6	1.541 (3)	C16—C17	1.390 (3)
C5—H5A	0.9700	C16—H16	0.9300
C5—H5B	0.9700	C17—C18	1.370 (4)
C6—C8	1.503 (3)	C17—H17	0.9300
C6—C7	1.556 (3)	C18—C19	1.369 (3)
C6—H6	0.9800	C18—H18	0.9300
C7—N1	1.462 (3)	C19—C20	1.382 (3)
C7—C15	1.510 (3)	C19—Cl2	1.742 (3)
C7—H7	0.9800	C20—H20	0.9300
C8—O1	1.218 (2)	N1—H1A	0.83 (2)
N1—C1—C9	111.35 (16)	O1—C8—C2	124.5 (2)
N1—C1—C2	108.66 (16)	O1—C8—C6	123.3 (2)
C9—C1—C2	113.05 (16)	C2—C8—C6	112.28 (17)
N1—C1—H1	107.9	C10—C9—C14	118.52 (19)

C9—C1—H1	107.9	C10—C9—C1	122.25 (18)
C2—C1—H1	107.9	C14—C9—C1	119.23 (18)
C8—C2—C3	107.59 (18)	C9—C10—C11	120.9 (2)
C8—C2—C1	107.01 (16)	C9—C10—H10	119.5
C3—C2—C1	116.25 (17)	C11—C10—H10	119.5
C8—C2—H2	108.6	C12—C11—C10	120.3 (2)
C3—C2—H2	108.6	C12—C11—H11	119.8
C1—C2—H2	108.6	C10—C11—H11	119.8
C4—C3—C2	113.96 (17)	C13—C12—C11	118.6 (2)
C4—C3—H3A	108.8	C13—C12—H12	120.7
C2—C3—H3A	108.8	C11—C12—H12	120.7
C4—C3—H3B	108.8	C12—C13—C14	121.8 (2)
C2—C3—H3B	108.8	C12—C13—Cl1	119.18 (17)
H3A—C3—H3B	107.7	C14—C13—Cl1	118.97 (16)
C5—C4—C3	112.78 (19)	C13—C14—C9	119.79 (19)
C5—C4—H4A	109.0	C13—C14—H14	120.1
C3—C4—H4A	109.0	C9—C14—H14	120.1
C5—C4—H4B	109.0	C16—C15—C20	118.3 (2)
C3—C4—H4B	109.0	C16—C15—C7	119.01 (19)
H4A—C4—H4B	107.8	C20—C15—C7	122.72 (18)
C4—C5—C6	114.49 (17)	C15—C16—C17	120.4 (2)
C4—C5—H5A	108.6	C15—C16—H16	119.8
C6—C5—H5A	108.6	C17—C16—H16	119.8
C4—C5—H5B	108.6	C18—C17—C16	120.8 (2)
C6—C5—H5B	108.6	C18—C17—H17	119.6
H5A—C5—H5B	107.6	C16—C17—H17	119.6
C8—C6—C5	107.32 (17)	C19—C18—C17	118.7 (2)
C8—C6—C7	106.25 (16)	C19—C18—H18	120.6
C5—C6—C7	116.39 (17)	C17—C18—H18	120.6
C8—C6—H6	108.9	C18—C19—C20	121.5 (2)
C5—C6—H6	108.9	C18—C19—Cl2	119.17 (19)
C7—C6—H6	108.9	C20—C19—Cl2	119.36 (18)
N1—C7—C15	111.44 (16)	C19—C20—C15	120.3 (2)
N1—C7—C6	109.14 (16)	C19—C20—H20	119.9
C15—C7—C6	112.37 (16)	C15—C20—H20	119.9
N1—C7—H7	107.9	C7—N1—C1	112.88 (15)
C15—C7—H7	107.9	C7—N1—H1A	108.0 (14)
C6—C7—H7	107.9	C1—N1—H1A	113.0 (14)

N1—C1—C2—C8	58.1 (2)	C1—C9—C10—C11	179.1 (2)
C9—C1—C2—C8	−177.77 (16)	C9—C10—C11—C12	0.2 (4)
N1—C1—C2—C3	−62.1 (2)	C10—C11—C12—C13	0.8 (4)
C9—C1—C2—C3	62.0 (2)	C11—C12—C13—C14	−1.3 (3)
C8—C2—C3—C4	−53.3 (2)	C11—C12—C13—Cl1	177.49 (19)
C1—C2—C3—C4	66.6 (3)	C12—C13—C14—C9	0.9 (3)
C2—C3—C4—C5	45.2 (3)	Cl1—C13—C14—C9	−177.89 (16)
C3—C4—C5—C6	−45.3 (3)	C10—C9—C14—C13	0.0 (3)
C4—C5—C6—C8	52.9 (2)	C1—C9—C14—C13	−179.61 (17)

C4—C5—C6—C7	−65.9 (2)	N1—C7—C15—C16	143.69 (19)
C8—C6—C7—N1	−58.4 (2)	C6—C7—C15—C16	−93.5 (2)
C5—C6—C7—N1	60.9 (2)	N1—C7—C15—C20	−37.3 (3)
C8—C6—C7—C15	177.42 (16)	C6—C7—C15—C20	85.5 (2)
C5—C6—C7—C15	−63.2 (2)	C20—C15—C16—C17	−1.1 (3)
C3—C2—C8—O1	−116.6 (2)	C7—C15—C16—C17	177.9 (2)
C1—C2—C8—O1	117.8 (2)	C15—C16—C17—C18	0.7 (4)
C3—C2—C8—C6	63.9 (2)	C16—C17—C18—C19	−0.3 (4)
C1—C2—C8—C6	−61.7 (2)	C17—C18—C19—C20	0.5 (4)
C5—C6—C8—O1	117.0 (2)	C17—C18—C19—Cl2	−179.20 (19)
C7—C6—C8—O1	−117.9 (2)	C18—C19—C20—C15	−1.0 (4)
C5—C6—C8—C2	−63.6 (2)	Cl2—C19—C20—C15	178.72 (16)
C7—C6—C8—C2	61.6 (2)	C16—C15—C20—C19	1.3 (3)
N1—C1—C9—C10	36.4 (3)	C7—C15—C20—C19	−177.8 (2)
C2—C1—C9—C10	−86.3 (2)	C15—C7—N1—C1	−174.09 (16)
N1—C1—C9—C14	−143.97 (18)	C6—C7—N1—C1	61.2 (2)
C2—C1—C9—C14	93.4 (2)	C9—C1—N1—C7	174.24 (16)
C14—C9—C10—C11	−0.6 (3)	C2—C1—N1—C7	−60.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.83 (2)	2.35 (2)	3.129 (3)	155.4 (18)
C7—H7···O1^{ii}	0.98	2.44	3.296 (2)	146

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*+1/2, −*y*+3/2, −*z*+2.