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

P. Parthiban,^a V. Ramkumar,^b H. D. Santan,^a Jong Tae Kim^a and Yeon Tae Jeong^{a*}^aDivision of Image Science and Information Engineering, Pukyong National University, Busan 608 739, Republic of Korea, and ^bDepartment of Chemistry, IIT Madras, Chennai, TamilNadu, India

Correspondence e-mail: ytjeong@pknu.ac.kr

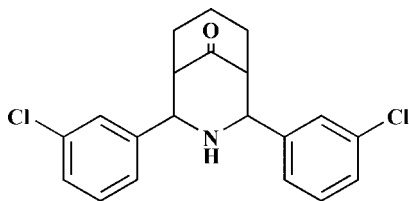
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.041; wR factor = 0.084; data-to-parameter ratio = 19.4.

In the molecular structure of the title compound, $\text{C}_{20}\text{H}_{19}\text{Cl}_2\text{NO}$, the bicyclic system adopts a twin-chair conformation with equatorial orientations of both substituents. The dihedral angle between the aromatic rings is $43.60(2)^\circ$ with respect to each other. The crystal structure is stabilized by weak $\text{N}-\text{H}\cdots\text{O}$ and strong $\text{C}-\text{H}\cdots\text{O}$ interactions.

Related literature

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



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{19}\text{Cl}_2\text{NO}$ $M_r = 360.26$ Orthorhombic, $P2_12_12_1$ $a = 6.9950(14)$ Å $b = 12.180(2)$ Å $c = 20.770(4)$ Å $V = 1769.6(6)$ Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.37$ mm⁻¹ $T = 298$ K $0.31 \times 0.25 \times 0.22$ 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 $I > 2\sigma(I)$ $R_{\text{int}} = 0.046$

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

 $\Delta\rho_{\text{max}} = 0.16$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Absolute structure: Flack (1983),

1756 Friedel pairs

Flack parameter: $-0.05(5)$

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O1}^i$	0.83 (2)	2.35 (2)	3.129 (3)	155.4 (18)
$\text{C7}-\text{H7}\cdots\text{O1}^{\text{ii}}$	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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supporting information

Acta Cryst. (2009). E65, 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 $C_{20}H_{19}Cl_2NO$, 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) $^\circ$, 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, $\theta = 2.71$ (19) $^\circ$. (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) $^\circ$, respectively, $Q_T = 0.562$ (2) Å, $q(2) = 0.128$ (2) and $q(3) = 0.549$ (2) Å, $\theta = 12.7$ (2) $^\circ$. (Cremer & Pople, 1975). The aryl groups are oriented at an angle of 43.60 (2) $^\circ$ to each other.

The crystal structure is stabilized by weak N—H \cdots O (3.129 (3)Å) and strong C—H \cdots O interactions [C1—H \cdots O1 (3.46 (3)Å) and C7—H \cdots 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 = 0.98 Å and methylen C—H = 0.97 Å. The displacement parameters were set for phenyl, methylen and aliphatic H atoms at $U_{iso}(H) = 1.2U_{eq}(C)$.

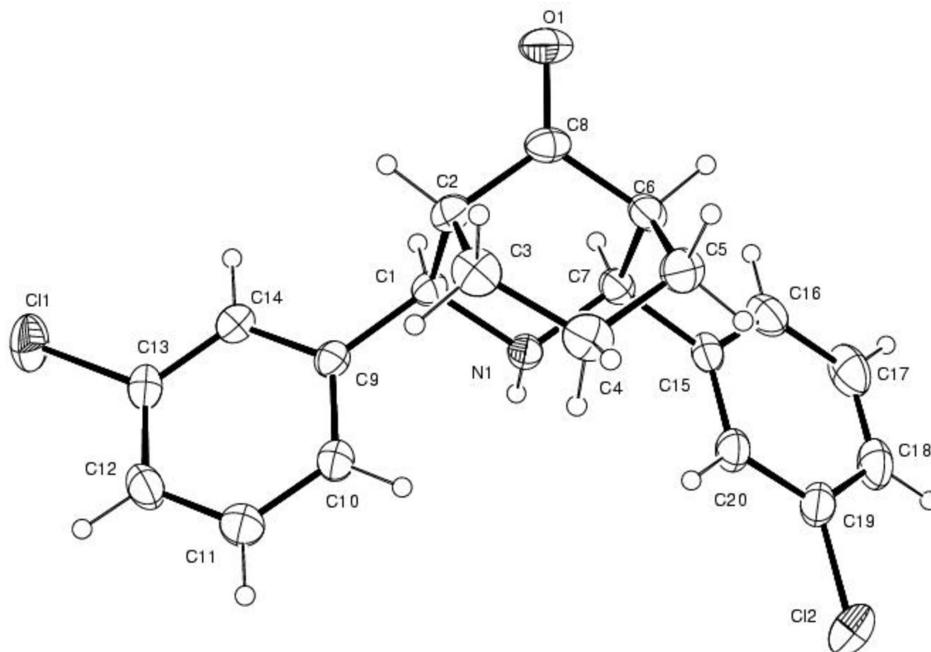


Figure 1

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

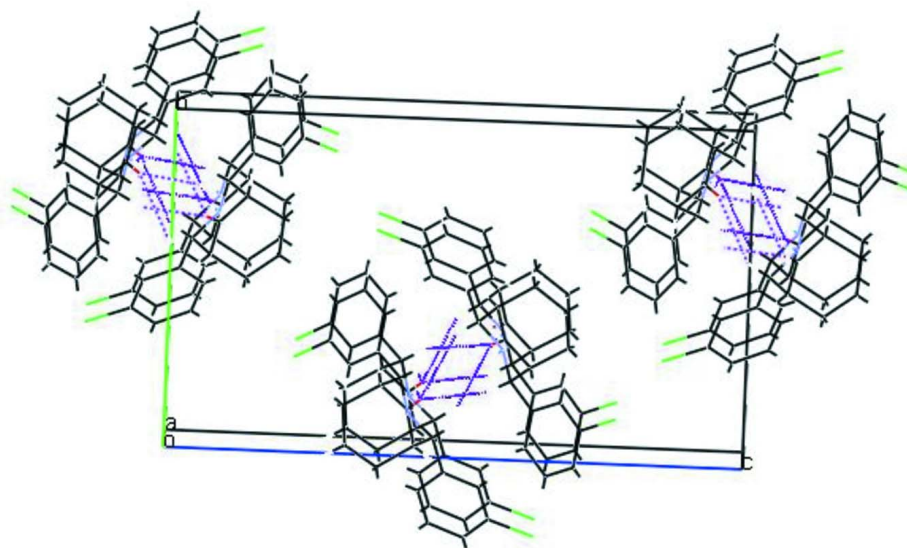


Figure 2

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

$a = 6.9950 (14) \text{ \AA}$

$b = 12.180 (2) \text{ \AA}$

$c = 20.770 (4) \text{ \AA}$

$V = 1769.6 (6) \text{ \AA}^3$

$Z = 4$

$F(000) = 752$

$D_x = 1.352 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 5421 reflections
 $\theta = 2.6\text{--}22.5^\circ$

$\mu = 0.37 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Block, colourless
 $0.31 \times 0.25 \times 0.22 \text{ mm}$

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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.046$
 $\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 2.6^\circ$
 $h = -8 \rightarrow 9$
 $k = -16 \rightarrow 16$
 $l = -27 \rightarrow 16$

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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.25 \text{ e \AA}^{-3}$
 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	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)
C11	0.0959 (5)	0.0649 (4)	0.0435 (3)	-0.0048 (4)	-0.0084 (3)	-0.0171 (3)
C12	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, °)

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—C11	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—C12	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—C11	119.18 (17)
H3A—C3—H3B	107.7	C14—C13—C11	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—C12	119.17 (19)
C7—C6—H6	108.9	C20—C19—C12	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—C11	177.49 (19)
C1—C2—C3—C4	66.6 (3)	C12—C13—C14—C9	0.9 (3)
C2—C3—C4—C5	45.2 (3)	C11—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—C12	-179.20 (19)
C7—C6—C8—O1	-117.9 (2)	C18—C19—C20—C15	-1.0 (4)
C5—C6—C8—C2	-63.6 (2)	C12—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 (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O1 ⁱ	0.83 (2)	2.35 (2)	3.129 (3)	155.4 (18)
C7—H7 \cdots O1 ⁱⁱ	0.98	2.44	3.296 (2)	146

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