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2,4-Bis(4-ethoxyphenyl)-7-methyl-3-azabicyclo[3.3.1]nonan-9-one

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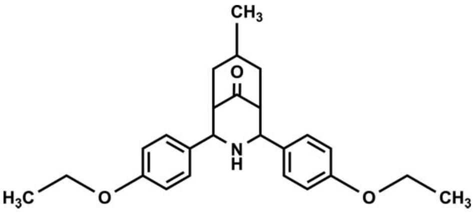
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.094; data-to-parameter ratio = 7.8.

The molecule of the title compound, $C_{25}H_{31}NO_3$, exists in a twin-chair conformation with an equatorial orientation of the 4-ethoxyphenyl groups, as observed for its *ortho* isomer [Parthiban, Ramkumar, Park & Jeong (2011*b*), *Acta Cryst.* E**67**, o1475–o1476]. The methyl and 4-ethoxyphenyl groups are also equatorially oriented on the bicycle, as in the *ortho* analogue. In particular, although the cyclohexanone ring deviates from an ideal chair, the piperidone ring is closer to an ideal chair, whereas in the *ortho* isomer both rings are significantly puckered and deviate from ideal chairs. The 4-ethoxyphenyl groups on both sides of the secondary amine group are oriented at an angle of 26.11 (3)° with respect to each other, but the 2-ethoxyphenyl groups in the *ortho* isomer are oriented by less than half this [12.41 (4)°]. In contrast to the absence of any significant interactions in the crystal packing of the *ortho* isomer, the title compound features N—H⋯O interactions, linking the molecules along the *b* axis.

Related literature

For the synthesis and stereochemistry of 3-azabicyclo[3.3.1]nonan-9-ones, see: Park *et al.* (2011). For the biological activities of 3-azabicyclo[3.3.1]nonan-9-ones, see: Barker *et al.* (2005); Parthiban *et al.* (2009, 2010*a*,*b*,2011*a*). For a related structure, see: Parthiban *et al.* (2011*b*). For ring-puckering parameters, see: Cremer & Pople (1975); Nardelli (1983).



Experimental

Crystal data

$C_{25}H_{31}NO_3$
M_r = 393.51
Orthorhombic, $Pmn2_1$
a = 19.329 (4) Å
b = 6.7967 (12) Å
c = 8.2501 (16) Å
V = 1083.8 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.35 × 0.28 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.973, T_{max} = 0.992
1565 measured reflections
1165 independent reflections
950 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 1.05
1165 reflections
150 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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}	0.86 (2)	2.26 (2)	3.073 (4)	158 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); 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: BQ2338).

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supplementary materials

Acta Cryst. (2012). E**68**, o779–o780 [doi:10.1107/S1600536812006563]

2,4-Bis(4-ethoxyphenyl)-7-methyl-3-azabicyclo[3.3.1]nonan-9-one

Dong Ho Park, V. Ramkumar and P. Parthiban

Comment

The 3-azabicyclononane nucleus is an important class of pharmacophore due to its broad-spectrum of biological actions ranging from antibacterial to anticancer (Barker *et al.*, 2005; Parthiban *et al.*, 2009, 2010*a*,*b*, 2011a). Owing to their broad-spectrum of biological actions, synthesis as well as isolaton of new molecules from the natural products, and their stereochemical analysis are considered as important in the field of medicinal chemistry. Hence, we synthesized the title compound by a modified and an optimized successive double Mannich condensation. Thus the obtained crystal was undertaken for this study to explore its stereochemistry in the solid-state.

The crystallographic parameters *viz.* torsion angles, asymmetry parameters and ring puckering parameters calculated for the title compound show that the piperidone ring adopts a near ideal chair conformation, according to Cremer & Pople and Nardelli (Fig. 1). The total puckering amplitude, Q_T is 0.607 (6) Å, the phase angle θ is 7.7 (6)° and φ is 180.0° (Cremer & Pople, 1975). The smallest displacement asymmetry parameters q_2 and q_3 are 0.081 (6) Å and 0.601 (6) Å, respectively (Nardelli, 1983). On the other hand, the cyclohexane ring deviates from the ideal chair conformation by Q_T = 0.536 (6), θ = 170.2 (7)° and φ = 240.0° (Cremer & Pople, 1975) as well as Nardelli by q_2 = 0.092 (7) and q_3 = 0.528 (6)° (Nardelli, 1983). In its *ortho* isomer, that is, 2,4-*bis*(2-ethoxyphenyl)-7-methyl-3-azabicyclo[3.3.1]nonan-9-one (Parthiban *et al.*, 2011b), both the piperidone and cyclohexanone rings deviated the ideal chair as follows (Q_T = 0.5889 (18), θ = 7.19 (18)° and Q_T = 0.554 (2), θ = 12.2 (2)°, respectively).

The aryl groups are orientated at an angle of 26.11 (3)° to each other. The center of symmetry passes through C6 C5 C3 N1 and O1. The torsion angle of C3—C2—C1—C7 and its mirror image is -176.7 (5)°. The angle with C&P plane normal of bonds C1—C7 as well as C1a—C7a and C5—C6 are 73.27 and 65.36 (2), respectively, conforms the equatorial disposition of the aryl and alkyl groups on the bicycle. Hence, the title compound $C_{25}H_{31}NO_3$, exists in a double-chair conformation with an equatorial orientation of the 4-ethoxyphenyl groups on both sides of the secondary amino group on the heterocycle and exocyclic orientation of the methyl on the cyclohexane ring.

The crystal packing is stabilized by an intermolecular N—H···O interaction of 2.26 (2) Å (Table 1 and Fig. 2).

Experimental

The 2,4-*bis*(4-ethoxyphenyl)-7-methyl-3-azabicyclo[3.3.1]nonan-9-one was synthesized by a modified and an optimized Mannich condensation in one-pot, using 4-ethoxybenzaldehyde (0.1 mol, 15.018 g/13.91 ml), cyclohexanone (0.05 mol, 5.61 g/6.14 ml) and ammonium acetate (0.075 mol, 5.78 g) in a 50 ml of absolute ethanol (Park *et al.*, 2001). The mixture was gently warmed on a hot plate at 303–308 K (30–35° C) with moderate stirring till the complete consumption of the starting materials, which was monitored by TLC. At the end, the crude azabicyclic ketone was separated by filtration and gently washed with 1:5 cold ethanol–ether mixture. X-ray diffraction quality crystals of the title compound were obtained by slow evaporation from ethanol.

Refinement

The nitrogen H atom and C6 H atoms were located by difference Fourier map and refined isotropically. Other H atoms were fixed geometrically and allowed to ride on the parent C atoms with aromatic C—H = 0.93 Å, aliphatic C—H = 0.98 Å and methylene C—H = 0.97 Å. The displacement parameters were set for phenyl, methylene and aliphatic H atoms at $U_{iso}(H) = 1.2U_{eq}(C)$ and for methyl H atoms at $U_{iso}(H) = 1.5U_{eq}(C)$. Because of the meaningless of the absolute structure parameter, 400 Friedel-pairs were merged before final refinement

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); 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* (Sheldrick, 2008).

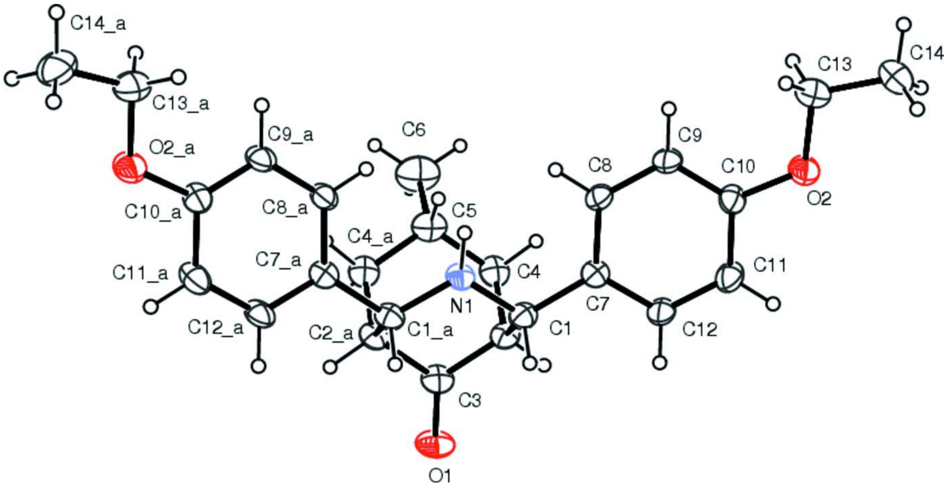

Figure 1

Molecular structure of the title compound showing the atom labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code for the half part of the molecule: -*x*, *y*, *z*.

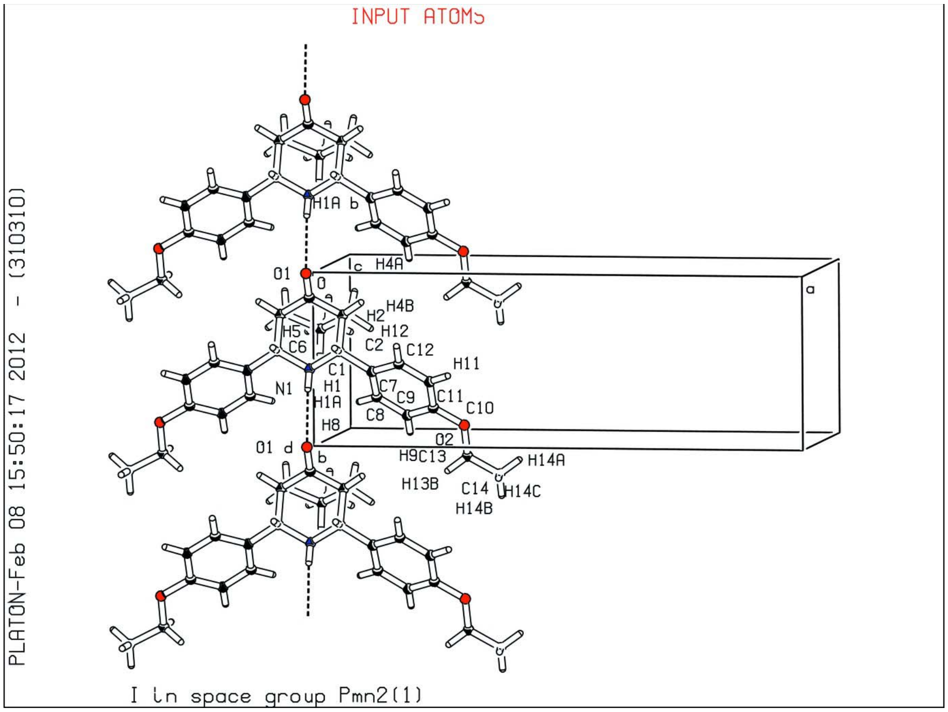

Figure 2

The packing of the title compound along *b*-axis. Dashed line shows intermolecular N—H···O H-bonds.

2,4-Bis(4-ethoxyphenyl)-7-methyl-3-azabicyclo[3.3.1]nonan-9-one

Crystal data

$C_{25}H_{31}NO_3$
$M_r = 393.51$
Orthorhombic, $Pmn2_1$
Hall symbol: P 2ac -2
$a = 19.329\ (4)$ Å
$b = 6.7967\ (12)$ Å
$c = 8.2501\ (16)$ Å
$V = 1083.8\ (4)$ Å^3
$Z = 2$

$F(000) = 424$
$D_x = 1.206$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1281 reflections
$\theta = 2.5–22.3°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Block, colourless
0.35 × 0.28 × 0.10 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, 2004)
$T_{\min} = 0.973$, $T_{\max} = 0.992$

1565 measured reflections
1165 independent reflections
950 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
$\theta_{\max} = 26.0°$, $\theta_{\min} = 2.1°$
$h = 0\rightarrow23$
$k = 0\rightarrow8$
$l = -7\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.094$
$S = 1.05$
1165 reflections
150 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.0596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.06340 (12)	0.4381 (3)	0.8529 (3)	0.0363 (6)
H1	0.0632	0.4085	0.7366	0.044*
C2	0.06391 (13)	0.2389 (3)	0.9456 (3)	0.0389 (6)
H2	0.1044	0.1628	0.9112	0.047*
C3	0.0000	0.1332 (5)	0.8932 (5)	0.0415 (8)
C4	0.06491 (14)	0.2575 (4)	1.1304 (3)	0.0477 (7)
H4A	0.0714	0.1276	1.1767	0.057*
H4B	0.1044	0.3370	1.1615	0.057*
C5	0.0000	0.3480 (6)	1.2034 (4)	0.0489 (10)
H5	0.0000	0.4887	1.1772	0.059*
C6	0.0000	0.3276 (10)	1.3882 (6)	0.0786 (15)
C7	0.12754 (11)	0.5559 (3)	0.8882 (3)	0.0349 (6)
C8	0.12963 (12)	0.7124 (4)	0.9938 (3)	0.0397 (6)
H8	0.0895	0.7477	1.0489	0.048*
C9	0.18980 (12)	0.8191 (4)	1.0205 (3)	0.0434 (6)
H9	0.1898	0.9248	1.0921	0.052*
C10	0.24949 (12)	0.7671 (4)	0.9402 (3)	0.0415 (6)
C11	0.24911 (14)	0.6067 (4)	0.8392 (4)	0.0517 (8)
H11	0.2898	0.5676	0.7885	0.062*
C12	0.18887 (13)	0.5027 (4)	0.8122 (4)	0.0463 (6)
H12	0.1893	0.3956	0.7421	0.056*
C13	0.31170 (14)	1.0533 (4)	1.0305 (4)	0.0610 (8)
H13A	0.3057	1.0357	1.1463	0.073*
H13B	0.2741	1.1343	0.9905	0.073*
C14	0.37939 (15)	1.1511 (5)	0.9972 (5)	0.0731 (10)

H14A	0.4162	1.0730	1.0414	0.110*
H14B	0.3798	1.2790	1.0466	0.110*
H14C	0.3856	1.1643	0.8823	0.110*
N1	0.0000	0.5455 (4)	0.8897 (4)	0.0361 (7)
O1	0.0000	−0.0133 (4)	0.8084 (4)	0.0603 (8)
O2	0.31106 (9)	0.8665 (3)	0.9511 (3)	0.0599 (6)
H1A	0.0000	0.656 (3)	0.840 (4)	0.033 (10)*
H6A	−0.0436 (13)	0.385 (5)	1.427 (5)	0.091 (12)*
H6B	0.0000	0.189 (4)	1.421 (7)	0.089 (18)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0373 (14)	0.0399 (13)	0.0318 (12)	0.0017 (10)	0.0031 (10)	0.0015 (11)
C2	0.0344 (13)	0.0350 (12)	0.0471 (13)	0.0070 (10)	0.0024 (12)	0.0050 (13)
C3	0.050 (2)	0.0315 (18)	0.0426 (18)	0.000	0.000	0.0048 (19)
C4	0.0452 (17)	0.0520 (15)	0.0459 (14)	−0.0029 (12)	−0.0086 (12)	0.0147 (14)
C5	0.057 (3)	0.053 (2)	0.0369 (18)	0.000	0.000	0.005 (2)
C6	0.095 (4)	0.103 (4)	0.038 (2)	0.000	0.000	0.008 (3)
C7	0.0319 (13)	0.0376 (13)	0.0353 (12)	0.0030 (10)	0.0060 (10)	0.0055 (12)
C8	0.0310 (12)	0.0453 (13)	0.0428 (13)	0.0050 (10)	0.0055 (10)	−0.0038 (13)
C9	0.0406 (14)	0.0435 (13)	0.0461 (13)	0.0031 (11)	0.0023 (12)	−0.0054 (14)
C10	0.0334 (13)	0.0414 (13)	0.0498 (13)	−0.0003 (11)	0.0052 (12)	−0.0004 (13)
C11	0.0369 (15)	0.0466 (15)	0.0717 (19)	0.0010 (12)	0.0197 (14)	−0.0083 (16)
C12	0.0442 (16)	0.0390 (13)	0.0556 (14)	0.0017 (12)	0.0131 (12)	−0.0078 (14)
C13	0.0543 (18)	0.0615 (18)	0.0672 (19)	−0.0074 (13)	0.0053 (15)	−0.0171 (18)
C14	0.065 (2)	0.076 (2)	0.079 (2)	−0.0226 (17)	0.0056 (18)	−0.021 (2)
N1	0.0317 (16)	0.0324 (16)	0.0441 (16)	0.000	0.000	0.0075 (14)
O1	0.073 (2)	0.0366 (14)	0.0713 (18)	0.000	0.000	−0.0071 (16)
O2	0.0388 (10)	0.0547 (11)	0.0862 (14)	−0.0084 (9)	0.0101 (10)	−0.0158 (13)

Geometric parameters (Å, º)

C1—N1	1.458 (3)	C8—C9	1.388 (3)
C1—C7	1.504 (3)	C8—H8	0.9300
C1—C2	1.555 (3)	C9—C10	1.376 (3)
C1—H1	0.9800	C9—H9	0.9300
C2—C3	1.493 (3)	C10—O2	1.371 (3)
C2—C4	1.530 (4)	C10—C11	1.373 (4)
C2—H2	0.9800	C11—C12	1.380 (3)
C3—O1	1.216 (4)	C11—H11	0.9300
C3—C2^{i}	1.493 (3)	C12—H12	0.9300
C4—C5	1.521 (4)	C13—O2	1.429 (3)
C4—H4A	0.9700	C13—C14	1.493 (4)
C4—H4B	0.9700	C13—H13A	0.9700
C5—C4^{i}	1.521 (4)	C13—H13B	0.9700
C5—C6	1.531 (6)	C14—H14A	0.9600
C5—H5	0.9800	C14—H14B	0.9600
C6—H6A	0.980 (18)	C14—H14C	0.9600
C6—H6B	0.98 (2)	N1—C1^{i}	1.458 (3)

C7—C8	1.375 (3)	N1—H1A	0.855 (18)
C7—C12	1.389 (3)		

N1—C1—C7	112.68 (19)	C12—C7—C1	118.5 (2)
N1—C1—C2	109.8 (2)	C7—C8—C9	122.0 (2)
C7—C1—C2	111.28 (19)	C7—C8—H8	119.0
N1—C1—H1	107.6	C9—C8—H8	119.0
C7—C1—H1	107.6	C10—C9—C8	119.4 (2)
C2—C1—H1	107.6	C10—C9—H9	120.3
C3—C2—C4	109.8 (2)	C8—C9—H9	120.3
C3—C2—C1	105.8 (2)	O2—C10—C11	115.8 (2)
C4—C2—C1	114.7 (2)	O2—C10—C9	124.7 (2)
C3—C2—H2	108.8	C11—C10—C9	119.5 (2)
C4—C2—H2	108.8	C10—C11—C12	120.6 (2)
C1—C2—H2	108.8	C10—C11—H11	119.7
O1—C3—C2	124.08 (16)	C12—C11—H11	119.7
O1—C3—C2^{i}	124.08 (16)	C11—C12—C7	120.9 (3)
C2—C3—C2^{i}	111.6 (3)	C11—C12—H12	119.5
C5—C4—C2	114.6 (2)	C7—C12—H12	119.5
C5—C4—H4A	108.6	O2—C13—C14	108.6 (2)
C2—C4—H4A	108.6	O2—C13—H13A	110.0
C5—C4—H4B	108.6	C14—C13—H13A	110.0
C2—C4—H4B	108.6	O2—C13—H13B	110.0
H4A—C4—H4B	107.6	C14—C13—H13B	110.0
C4^{i}—C5—C4	111.1 (3)	H13A—C13—H13B	108.3
C4^{i}—C5—C6	110.9 (2)	C13—C14—H14A	109.5
C4—C5—C6	110.9 (2)	C13—C14—H14B	109.5
C4^{i}—C5—H5	107.9	H14A—C14—H14B	109.5
C4—C5—H5	107.9	C13—C14—H14C	109.5
C6—C5—H5	107.9	H14A—C14—H14C	109.5
C5—C6—H6A	107 (3)	H14B—C14—H14C	109.5
C5—C6—H6B	111 (4)	C1^{i}—N1—C1	114.3 (3)
H6A—C6—H6B	107 (3)	C1^{i}—N1—H1A	109.9 (10)
C8—C7—C12	117.5 (2)	C1—N1—H1A	109.9 (10)
C8—C7—C1	124.0 (2)	C10—O2—C13	118.37 (19)

N1—C1—C2—C3	57.5 (3)	C12—C7—C8—C9	2.2 (4)
C7—C1—C2—C3	−177.0 (2)	C1—C7—C8—C9	−178.9 (2)
N1—C1—C2—C4	−63.6 (3)	C7—C8—C9—C10	−0.4 (4)
C7—C1—C2—C4	61.9 (3)	C8—C9—C10—O2	176.9 (2)
C4—C2—C3—O1	−125.3 (4)	C8—C9—C10—C11	−2.1 (4)
C1—C2—C3—O1	110.4 (4)	O2—C10—C11—C12	−176.3 (3)
C4—C2—C3—C2^{i}	59.6 (4)	C9—C10—C11—C12	2.8 (4)
C1—C2—C3—C2^{i}	−64.7 (3)	C10—C11—C12—C7	−1.0 (4)
C3—C2—C4—C5	−53.1 (3)	C8—C7—C12—C11	−1.5 (4)
C1—C2—C4—C5	65.9 (3)	C1—C7—C12—C11	179.5 (2)
C2—C4—C5—C4^{i}	46.1 (4)	C7—C1—N1—C1^{i}	178.43 (16)
C2—C4—C5—C6	170.0 (3)	C2—C1—N1—C1^{i}	−56.9 (3)
N1—C1—C7—C8	22.0 (3)	C11—C10—O2—C13	169.0 (3)

C2—C1—C7—C8	−101.9 (3)	C9—C10—O2—C13	−10.0 (4)
N1—C1—C7—C12	−159.1 (2)	C14—C13—O2—C10	−168.2 (3)
C2—C1—C7—C12	77.1 (3)		

Symmetry code: (i) −*x*, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{ii}	0.86 (2)	2.26 (2)	3.073 (4)	158 (3)

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