organic compounds

Benzyl N-{2-[5-(4-chlorophenyl)-1,2,4-oxadiazol-3-yl]propan-2-yl}carbamate

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In the title 1,2,4-oxadiazole derivative, $C_{19}H_{18}ClN_3O_3$, the 1,2,4-oxadiazole ring makes dihedral angles of 12.83 (8) and 4.89 (8)°, respectively, with the benzyl and 4-chlorophenyl rings, while the dihedral angle between the benzyl and 4-chlorophenyl rings is 11.53 (7)°. In the crystal, molecules are linked by N—H⋯N hydrogen bonds into helical chains along the b axis. A weak C—H⋯π interaction is also present.

Related literature

For bond-length data, see: Allen et al. (1987). For background to and applications of 1,2,4-oxadiazole derivatives, see: Chen et al. (1994); Chimirri et al. (1996); Clitherow et al. (1996); Nicolaides et al. (1998); Saunders et al. (1990); Showell et al. (1991); Swain et al. (1991); Tully et al. (1991); Watjen et al. (1989). For a related structure, see: Fun et al. (2011).
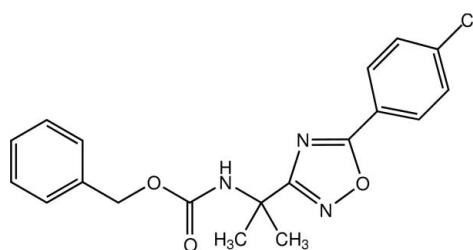
Experimental

Crystal data

$C_{19}H_{18}ClN_3O_3$
M_r = 371.81

Orthorhombic, $P2_12_12_1$
a = 7.7501 (1) Å

b = 11.0052 (2) Å
c = 20.9834 (3) Å
V = 1789.70 (5) Å^3
Z = 4

Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 297 K
0.41 × 0.35 × 0.21 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2005)
T_{min} = 0.908, T_{max} = 0.951

15995 measured reflections
4556 independent reflections
3620 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.087
S = 1.02
4556 reflections
241 parameters
H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1950 Friedel pairs
Flack parameter: 0.01 (6)

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

Cg1 is the centroid of the C12–C17 ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N3—H1N3⋯N2[i]	0.840 (16)	2.428 (15)	3.2492 (18)	165.7 (14)
C16—H16A⋯Cg1[ii]	0.93	2.91	3.6700 (18)	140

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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supporting information

Benzyl *N*-{2-[5-(4-chlorophenyl)-1,2,4-oxadiazol-3-yl]propan-2-yl}carbamate

Hoong-Kun Fun, V. Sumangala, G. K. Nagaraja, Boja Poojary and Suchada Chantrapromma

S1. Comment

The 1,2,4-oxadiazole ring occurs frequently in biologically active synthetic compounds and 1,2,4-oxadiazole derivatives are suggested as potential agonists for cortical muscarinic (Saunders *et al.*, 1990; Showell *et al.*, 1991), benzodiazepine (Watjen *et al.*, 1989; Tully *et al.*, 1991) and 5-HT1D (5-hydroxytryptamine) as receptors (Chen *et al.*, 1994) as well as antagonists for 5-HT3 (Swain *et al.*, 1991) or histamine H3 receptors (Clitherow *et al.*, 1996). They also demonstrate anti-inflammatory (Nicolaides *et al.*, 1998) and antitumor activities (Chimirri *et al.*, 1996). These interesting and important properties of 1,2,4-oxadiazole derivatives lead us to synthesize the title compound (I) and its crystal structure was reported.

In the molecule of (I), (Fig. 1), the 1,2,4-oxadiazole ring is nearly co-planar with the 4-chlorophenyl with a dihedral angle between the two rings being 4.89 (8)°, whereas it is inclined to the benzyl (C11–C17) unit with a dihedral angle of 12.48 (9)°. The dihedral angle between the benzyl group and the phenyl (C1–C6) ring is 11.53 (7)°. The oxycarbonyl-amino unit (atoms C10, N3, O2 and O3) is planar with an *r.m.s.* 0.0009 (1) Å. This unit makes dihedral angles of 79.99 (9), 89.15 (9) and 89.64 (9)°, respectively, with the benzyl, 1,2,4-oxadiazole and 4-chlorophenyl rings. The bond distances are of normal values (Allen *et al.*, 1987) and are comparable to the related structure (Fun *et al.*, 2011).

In the crystal packing (Fig. 2), the molecules are linked by by N—H···N hydrogen bonds (Table 1) into helical chains along the *b* axis. The crystal is stabilized by N—H···O hydrogen bonds and weak C—H···π interactions (Table 1).

S2. Experimental

The title compound was synthesized by taking benzyl [(2*E*)-2-amino-2-(hydroxyimino)-1,1-dimethylethyl]carbamate (0.1 mole) in 5 mol volume of pyridine and treated with 0.1 mole of 4-chlorobenzoylchloride. The reaction mixture is heated to reflux for 3–4 hrs. After the reaction is completed, the excess pyridine is distilled out under low pressure and the resultant quenched onto ice water. The solid thus formed is filtered and washed with water. The sample is dried and recrystallized in ethanol yielding 95% product. Colorless plate-shaped single crystals of the title compound suitable for *x*-ray structure determination were recrystalized from ethanol by the slow evaporation of the solvent at room temperature after several days (m.p. 405–409 K).

S3. Refinement

NH hydrogen atom is located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with *d*(C—H) = 0.93 Å for aromatic and 0.96 Å for CH$_3$ atoms. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. A total of 1950 Friedel pairs were used to determined the absolute configuration
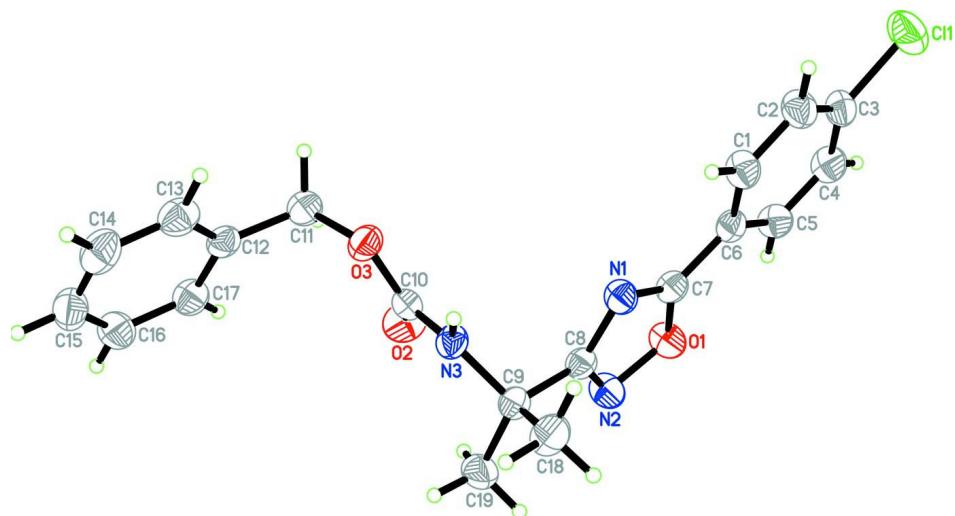
Figure 1

The molecular structure of the title compound, showing 40% probability displacement ellipsoids and the atom-numbering scheme.
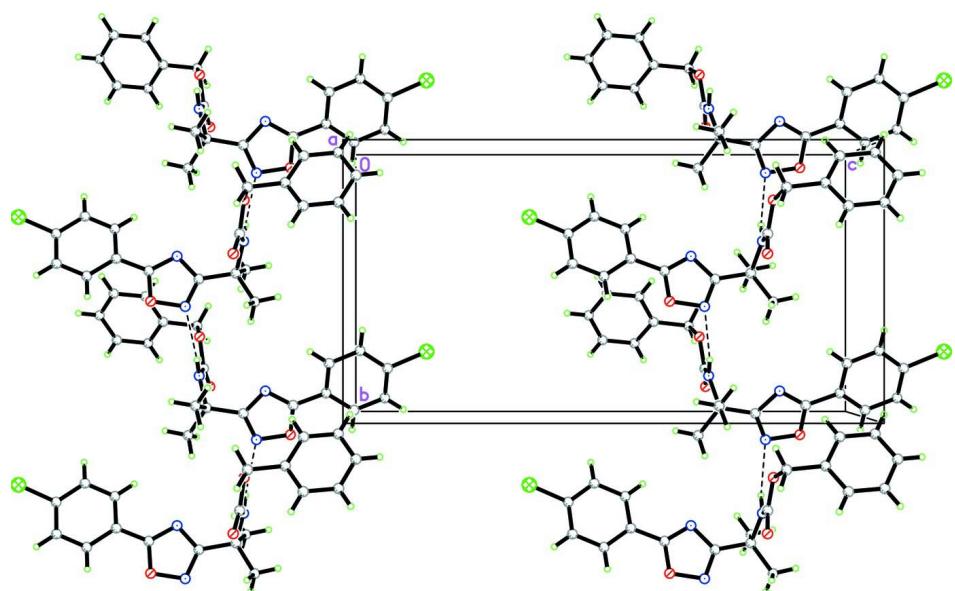
Figure 2

The crystal packing of the title compound viewed along the *a* axis, showing helical chains along the *b* axis. N—H⋯N hydrogen bonds are shown as dashed lines.

Benzyl *N*-{2-[5-(4-chlorophenyl)-1,2,4-oxadiazol-3-yl]propan-2-yl}carbamate

Crystal data

$C_{19}H_{18}ClN_3O_3$	$c = 20.9834 (3)$ Å
$M_r = 371.81$	$V = 1789.70 (5)$ Å^3
Orthorhombic, $P2_12_12_1$	$Z = 4$
Hall symbol: P 2ac 2ab	$F(000) = 776$
$a = 7.7501 (1)$ Å	$D_x = 1.380$ Mg m^{-3}
$b = 11.0052 (2)$ Å	Melting point = 405–409 K

Mo *Kα* radiation, *λ* = 0.71073 Å

Cell parameters from 4556 reflections

θ = 1.9–28.5°

μ = 0.24 mm⁻¹

T = 297 K

Plate, colorless

0.41 × 0.35 × 0.21 mm

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: sealed tube

Graphite monochromator

φ and *ω* scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2005)

T_{min} = 0.908, T_{max} = 0.951

15995 measured reflections

4556 independent reflections

3620 reflections with $I > 2\sigma(I)$

R_{int} = 0.028

θ_{max} = 28.5°, θ_{min} = 1.9°

h = −10→8

k = −14→14

l = −23→28

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.036

$wR(F^2)$ = 0.087

S = 1.02

4556 reflections

241 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

$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 0.0092P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.14 e Å⁻³

$\Delta\rho_{min}$ = −0.21 e Å⁻³

Absolute structure: Flack (1983), 1950 Friedel
pairs

Absolute structure parameter: 0.01 (6)

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}
Cl1	1.06337 (9)	0.74415 (5)	−0.14993 (2)	0.08010 (19)
O1	0.90644 (16)	0.42996 (9)	0.11883 (5)	0.0490 (3)
O2	0.62272 (16)	0.60054 (11)	0.29142 (7)	0.0631 (4)
O3	0.71211 (14)	0.79437 (9)	0.30763 (6)	0.0501 (3)
N1	1.00418 (18)	0.59694 (10)	0.16396 (6)	0.0422 (3)
N2	0.89957 (19)	0.41084 (11)	0.18577 (6)	0.0487 (3)
N3	0.90781 (17)	0.65050 (11)	0.29774 (6)	0.0401 (3)
C1	1.0718 (2)	0.70094 (14)	0.03799 (7)	0.0470 (4)
H1A	1.1094	0.7446	0.0733	0.056*
C2	1.0945 (2)	0.74801 (15)	−0.02232 (8)	0.0522 (4)
H2A	1.1470	0.8233	−0.0279	0.063*

C3	1.0385 (2)	0.68209 (16)	−0.07420 (7)	0.0499 (4)
C4	0.9627 (2)	0.56952 (14)	−0.06747 (8)	0.0517 (4)
H4A	0.9283	0.5255	−0.1031	0.062*
C5	0.9386 (2)	0.52308 (13)	−0.00694 (7)	0.0469 (4)
H5A	0.8859	0.4478	−0.0017	0.056*
C6	0.9930 (2)	0.58868 (12)	0.04632 (7)	0.0393 (3)
C7	0.96954 (19)	0.54258 (12)	0.11114 (7)	0.0386 (3)
C8	0.9582 (2)	0.51195 (12)	0.20882 (7)	0.0371 (3)
C9	0.9872 (2)	0.53376 (12)	0.27932 (7)	0.0417 (4)
C10	0.7365 (2)	0.67374 (13)	0.29808 (7)	0.0414 (3)
C11	0.5372 (2)	0.83404 (16)	0.32187 (8)	0.0528 (4)
H11A	0.4552	0.7744	0.3064	0.063*
H11B	0.5141	0.9106	0.3007	0.063*
C12	0.51699 (19)	0.84918 (13)	0.39282 (7)	0.0423 (3)
C13	0.5898 (2)	0.94799 (14)	0.42406 (9)	0.0545 (4)
H13A	0.6480	1.0070	0.4008	0.065*
C14	0.5766 (3)	0.95920 (16)	0.48927 (9)	0.0621 (5)
H14A	0.6270	1.0253	0.5096	0.074*
C15	0.4903 (3)	0.87436 (17)	0.52416 (9)	0.0591 (5)
H15A	0.4826	0.8825	0.5682	0.071*
C16	0.4146 (2)	0.77656 (16)	0.49429 (8)	0.0572 (4)
H16A	0.3541	0.7191	0.5179	0.069*
C17	0.4292 (2)	0.76457 (13)	0.42877 (8)	0.0496 (4)
H17A	0.3788	0.6981	0.4087	0.060*
C18	1.1805 (2)	0.54871 (16)	0.28978 (9)	0.0562 (5)
H18A	1.2220	0.6155	0.2647	0.084*
H18B	1.2389	0.4756	0.2773	0.084*
H18C	1.2024	0.5645	0.3340	0.084*
C19	0.9170 (3)	0.42786 (14)	0.31875 (8)	0.0592 (5)
H19A	0.7970	0.4162	0.3092	0.089*
H19B	0.9302	0.4456	0.3633	0.089*
H19C	0.9799	0.3552	0.3085	0.089*
H1N3	0.973 (2)	0.7115 (14)	0.2985 (7)	0.036 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1106 (5)	0.0857 (4)	0.0440 (2)	0.0012 (3)	0.0132 (3)	0.0075 (2)
O1	0.0635 (7)	0.0416 (5)	0.0418 (6)	−0.0124 (5)	−0.0050 (6)	−0.0044 (4)
O2	0.0508 (7)	0.0552 (7)	0.0833 (10)	−0.0086 (6)	−0.0013 (7)	0.0010 (6)
O3	0.0486 (7)	0.0433 (5)	0.0584 (7)	0.0076 (5)	0.0118 (6)	0.0012 (5)
N1	0.0508 (8)	0.0373 (6)	0.0384 (7)	−0.0039 (5)	0.0004 (6)	−0.0046 (5)
N2	0.0609 (9)	0.0431 (7)	0.0422 (7)	−0.0097 (6)	−0.0013 (7)	−0.0010 (5)
N3	0.0438 (8)	0.0338 (6)	0.0425 (7)	−0.0013 (6)	0.0046 (6)	−0.0040 (5)
C1	0.0536 (10)	0.0451 (8)	0.0422 (8)	−0.0064 (7)	−0.0001 (8)	−0.0097 (6)
C2	0.0575 (10)	0.0478 (8)	0.0514 (9)	−0.0079 (8)	0.0081 (8)	−0.0012 (7)
C3	0.0530 (10)	0.0577 (9)	0.0389 (8)	0.0070 (8)	0.0062 (8)	−0.0006 (7)
C4	0.0598 (11)	0.0534 (9)	0.0420 (8)	0.0038 (8)	−0.0090 (8)	−0.0110 (7)

C5	0.0536 (11)	0.0415 (8)	0.0457 (8)	−0.0013 (7)	−0.0070 (8)	−0.0065 (6)
C6	0.0399 (8)	0.0388 (7)	0.0390 (8)	0.0034 (6)	0.0000 (7)	−0.0060 (5)
C7	0.0376 (8)	0.0352 (7)	0.0431 (8)	−0.0002 (6)	−0.0026 (7)	−0.0057 (6)
C8	0.0374 (8)	0.0328 (6)	0.0410 (7)	0.0000 (6)	0.0007 (6)	−0.0021 (5)
C9	0.0507 (10)	0.0357 (7)	0.0389 (8)	0.0043 (6)	0.0017 (7)	−0.0032 (6)
C10	0.0496 (9)	0.0419 (7)	0.0327 (7)	0.0033 (7)	0.0047 (7)	0.0044 (6)
C11	0.0474 (10)	0.0591 (10)	0.0518 (10)	0.0146 (8)	0.0031 (8)	0.0053 (7)
C12	0.0345 (8)	0.0425 (7)	0.0499 (9)	0.0088 (6)	0.0019 (7)	0.0026 (6)
C13	0.0503 (10)	0.0438 (8)	0.0692 (12)	−0.0025 (8)	0.0048 (9)	0.0023 (8)
C14	0.0618 (12)	0.0539 (10)	0.0705 (12)	0.0008 (9)	−0.0075 (11)	−0.0185 (8)
C15	0.0585 (12)	0.0680 (11)	0.0507 (10)	0.0107 (9)	0.0034 (9)	−0.0074 (8)
C16	0.0589 (11)	0.0567 (10)	0.0561 (10)	−0.0002 (9)	0.0101 (9)	0.0080 (7)
C17	0.0506 (10)	0.0423 (8)	0.0560 (9)	−0.0043 (8)	0.0001 (8)	−0.0035 (7)
C18	0.0540 (11)	0.0618 (10)	0.0528 (10)	0.0117 (8)	−0.0128 (9)	−0.0138 (8)
C19	0.0924 (15)	0.0401 (8)	0.0452 (9)	0.0039 (9)	0.0064 (10)	0.0028 (6)

Geometric parameters (Å, °)

Cl1—C3	1.7404 (16)	C8—C9	1.515 (2)
O1—C7	1.3422 (16)	C9—C18	1.523 (2)
O1—N2	1.4213 (17)	C9—C19	1.529 (2)
O2—C10	1.2023 (19)	C11—C12	1.506 (2)
O3—C10	1.3558 (18)	C11—H11A	0.9700
O3—C11	1.455 (2)	C11—H11B	0.9700
N1—C7	1.2877 (18)	C12—C17	1.378 (2)
N1—C8	1.3740 (19)	C12—C13	1.390 (2)
N2—C8	1.2955 (18)	C13—C14	1.378 (3)
N3—C10	1.352 (2)	C13—H13A	0.9300
N3—C9	1.4758 (18)	C14—C15	1.362 (3)
N3—H1N3	0.841 (16)	C14—H14A	0.9300
C1—C2	1.379 (2)	C15—C16	1.377 (3)
C1—C6	1.389 (2)	C15—H15A	0.9300
C1—H1A	0.9300	C16—C17	1.386 (2)
C2—C3	1.378 (2)	C16—H16A	0.9300
C2—H2A	0.9300	C17—H17A	0.9300
C3—C4	1.378 (2)	C18—H18A	0.9600
C4—C5	1.382 (2)	C18—H18B	0.9600
C4—H4A	0.9300	C18—H18C	0.9600
C5—C6	1.3957 (19)	C19—H19A	0.9600
C5—H5A	0.9300	C19—H19B	0.9600
C6—C7	1.463 (2)	C19—H19C	0.9600
C7—O1—N2	105.61 (10)	O2—C10—O3	124.84 (16)
C10—O3—C11	116.99 (13)	N3—C10—O3	108.82 (14)
C7—N1—C8	102.66 (12)	O3—C11—C12	109.46 (13)
C8—N2—O1	103.21 (11)	O3—C11—H11A	109.8
C10—N3—C9	125.11 (13)	C12—C11—H11A	109.8
C10—N3—H1N3	116.2 (10)	O3—C11—H11B	109.8

C9—N3—H1N3	116.6 (10)	C12—C11—H11B	109.8
C2—C1—C6	120.39 (14)	H11A—C11—H11B	108.2
C2—C1—H1A	119.8	C17—C12—C13	118.11 (15)
C6—C1—H1A	119.8	C17—C12—C11	121.18 (14)
C3—C2—C1	119.14 (15)	C13—C12—C11	120.70 (15)
C3—C2—H2A	120.4	C14—C13—C12	120.56 (16)
C1—C2—H2A	120.4	C14—C13—H13A	119.7
C2—C3—C4	121.76 (15)	C12—C13—H13A	119.7
C2—C3—Cl1	118.67 (13)	C15—C14—C13	120.61 (17)
C4—C3—Cl1	119.56 (13)	C15—C14—H14A	119.7
C3—C4—C5	118.97 (14)	C13—C14—H14A	119.7
C3—C4—H4A	120.5	C14—C15—C16	120.02 (18)
C5—C4—H4A	120.5	C14—C15—H15A	120.0
C4—C5—C6	120.26 (15)	C16—C15—H15A	120.0
C4—C5—H5A	119.9	C15—C16—C17	119.42 (16)
C6—C5—H5A	119.9	C15—C16—H16A	120.3
C1—C6—C5	119.47 (14)	C17—C16—H16A	120.3
C1—C6—C7	118.68 (13)	C12—C17—C16	121.27 (15)
C5—C6—C7	121.84 (14)	C12—C17—H17A	119.4
N1—C7—O1	113.68 (13)	C16—C17—H17A	119.4
N1—C7—C6	127.82 (13)	C9—C18—H18A	109.5
O1—C7—C6	118.50 (12)	C9—C18—H18B	109.5
N2—C8—N1	114.83 (13)	H18A—C18—H18B	109.5
N2—C8—C9	123.53 (13)	C9—C18—H18C	109.5
N1—C8—C9	121.50 (12)	H18A—C18—H18C	109.5
N3—C9—C8	109.39 (12)	H18B—C18—H18C	109.5
N3—C9—C18	106.14 (13)	C9—C19—H19A	109.5
C8—C9—C18	107.66 (13)	C9—C19—H19B	109.5
N3—C9—C19	111.94 (13)	H19A—C19—H19B	109.5
C8—C9—C19	110.79 (12)	C9—C19—H19C	109.5
C18—C9—C19	110.72 (15)	H19A—C19—H19C	109.5
O2—C10—N3	126.34 (14)	H19B—C19—H19C	109.5
C7—O1—N2—C8	−0.08 (16)	C10—N3—C9—C18	−177.07 (15)
C6—C1—C2—C3	−0.2 (3)	C10—N3—C9—C19	−56.2 (2)
C1—C2—C3—C4	−1.0 (3)	N2—C8—C9—N3	−131.00 (16)
C1—C2—C3—Cl1	178.49 (14)	N1—C8—C9—N3	53.48 (19)
C2—C3—C4—C5	1.6 (3)	N2—C8—C9—C18	114.08 (17)
Cl1—C3—C4—C5	−177.88 (13)	N1—C8—C9—C18	−61.44 (18)
C3—C4—C5—C6	−1.0 (3)	N2—C8—C9—C19	−7.1 (2)
C2—C1—C6—C5	0.7 (2)	N1—C8—C9—C19	177.35 (15)
C2—C1—C6—C7	−179.32 (15)	C9—N3—C10—O2	9.9 (3)
C4—C5—C6—C1	−0.1 (2)	C9—N3—C10—O3	−170.43 (13)
C4—C5—C6—C7	179.93 (15)	C11—O3—C10—O2	11.3 (2)
C8—N1—C7—O1	−0.38 (18)	C11—O3—C10—N3	−168.37 (12)
C8—N1—C7—C6	−179.60 (15)	C10—O3—C11—C12	98.05 (16)
N2—O1—C7—N1	0.30 (18)	O3—C11—C12—C17	−104.15 (17)
N2—O1—C7—C6	179.60 (13)	O3—C11—C12—C13	74.49 (18)

C1—C6—C7—N1	4.6 (2)	C17—C12—C13—C14	1.1 (2)
C5—C6—C7—N1	−175.44 (16)	C11—C12—C13—C14	−177.57 (16)
C1—C6—C7—O1	−174.60 (14)	C12—C13—C14—C15	−0.7 (3)
C5—C6—C7—O1	5.4 (2)	C13—C14—C15—C16	−0.3 (3)
O1—N2—C8—N1	−0.16 (18)	C14—C15—C16—C17	0.9 (3)
O1—N2—C8—C9	−175.95 (14)	C13—C12—C17—C16	−0.5 (2)
C7—N1—C8—N2	0.33 (19)	C11—C12—C17—C16	178.18 (15)
C7—N1—C8—C9	176.22 (14)	C15—C16—C17—C12	−0.5 (3)
C10—N3—C9—C8	67.03 (18)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C12–C17 ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N3—H1*N*3⋯N2[i]	0.840 (16)	2.428 (15)	3.2492 (18)	165.7 (14)
C16—H16*A*⋯*Cg*1[ii]	0.93	2.91	3.6700 (18)	140

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