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5,6-Dimethyl-2-[(5-methyl-1,2-oxazol-3-yl)methyl]-1-(prop-2-en-1-yl)-1*H*-1,3-benzodiazole

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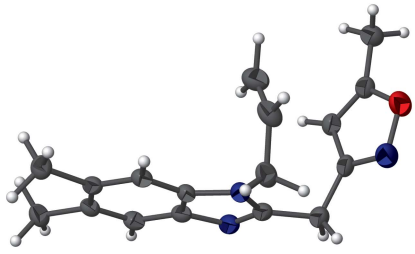
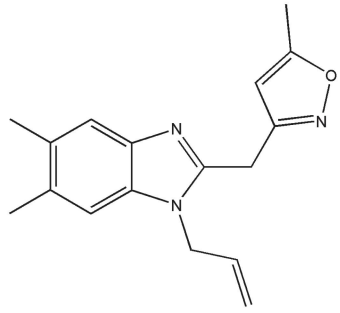
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{17}H_{19}N_3O$, the benzodiazole moiety is twisted slightly end-to-end. In the crystal, two sets of weak C—H···N hydrogen bonds form sheets approximately parallel to (100), which are formed into bilayers by pairwise C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

Benzimidazole derivatives have been shown to possess various biological activities including anti-histaminic (Al Muhaimeed, 1997) anti-ulcerative (Scott *et al.*, 2002) and anti-allergic (Nakano *et al.*, 2000). In addition, they are effective against the human cytomegalovirus (HCMV) (Zhu *et al.*, 2000) and are also efficient selective neuropeptide Y Y1 receptor antagonists (Zarrinmayeh *et al.*, 1998). Isoxazole derivatives represent a unique class of nitrogen and oxygen-containing five-membered heterocycles and are the components of a variety of natural products and medicinally useful compounds (Sperry & Wright, 2005). Isoxazole derivatives with a variety of substituents are known to have various biological activities in both the pharmaceutical and agricultural areas (Lang & Lin, 1984; Boyd, 1991). As a continuation of our previous studies (Sebbar *et al.*, 2015, 2016; El Azzaoui *et al.*, 2006), we were interested in the synthesis and the crystal structure of the title compound (Fig. 1).

The benzodiazole moiety is slightly non-planar, as indicated by the dihedral angle of 1.3 (1)° between the five- and six-membered rings. The oxazole ring is planar to within 0.005 (1) Å and makes a dihedral angle of 89.78 (8)° with the diazole ring.

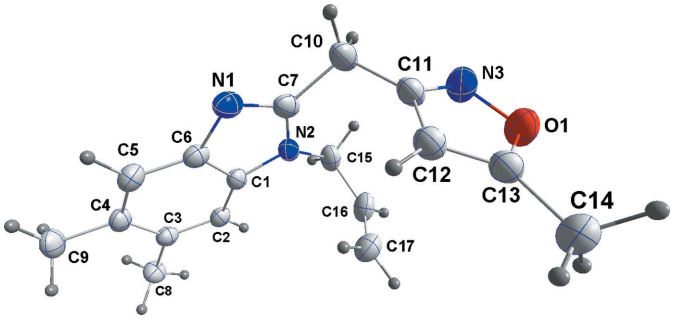


Figure 1
The title molecule with the labeling scheme and 50% probability ellipsoids.

In the crystal, weak C2—H2···N1($x, \frac{3}{2} - y, \frac{1}{2} + z$) hydrogen bonds link the molecules into chains running along the *c*-axis direction, which are joined into corrugated sheets by weak C12—H12···N3($x, -1 + y, z$) hydrogen bonds running approximately parallel to the *c*-axis direction (Table 1 and Figs. 2 and 3). The sheets are formed into bilayers through complementary C14—H14*A*···π(ring) interactions across centers of symmetry (Table 1 and Figs. 2 and 3).

Synthesis and crystallization

To a solution of 5,6-dimethyl-2-(5-methyl-isoxazol-3-yl)-methyl-1*H*-benzimidazole (4.3 mmol; 1.07 g) in *N*,*N*-dimethylformamide (20 ml) were added allyl bromide (4.5 mmol; 0.54 g), potassium carbonate (4.3 mmol) and a catalytic amount of tetra-*n*-butylammonium bromide. The reaction mixture was stirred at room temperature for 12 h. After cooling, the solid material was removed by filtration and the solvent evaporated in reduced pressure. The residue obtained was recrystallized from ethanol solution to afford the title compound as colourless crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

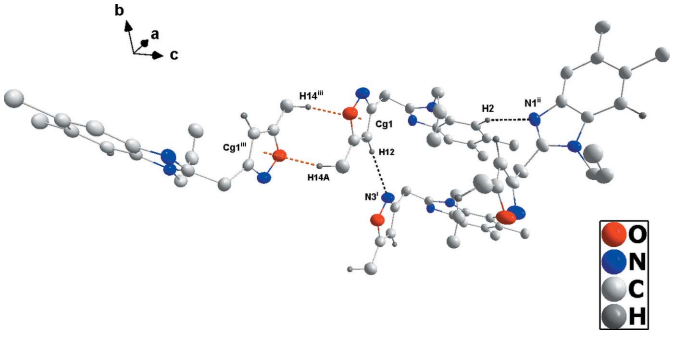


Figure 2
Detail of the C—H···N hydrogen bonds (black dotted lines) and the C—H···π(ring) interactions (orange dotted lines). Symmetry codes: (i) $x, -1 + y, z$; (ii) $x, \frac{3}{2} - y, \frac{1}{2} + z$; (iii) $1 - x, 2 - y, -z$).

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

Cg is the centroid of the N3/O1/C11–C13 oxazole ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N1^{i}	1.010 (19)	2.65 (2)	3.603 (2)	157.9 (15)
C12—H12···N3^{ii}	1.00 (2)	2.50 (3)	3.358 (3)	143.6 (17)
C14—H14*A*···*Cg*1^{iii}	1.01 (3)	2.77 (3)	3.704 (3)	154 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{19}N_3O$
M_r	281.35
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	19.6067 (6), 5.5438 (2), 14.0069 (5)
β (°)	99.911 (2)
V (Å^3)	1499.77 (9)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.63
Crystal size (mm)	0.12 × 0.07 × 0.01
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.86, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10867, 2825, 2121
R_{int}	0.059
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.609
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.111, 1.05
No. of reflections	2825
No. of parameters	267
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.23

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

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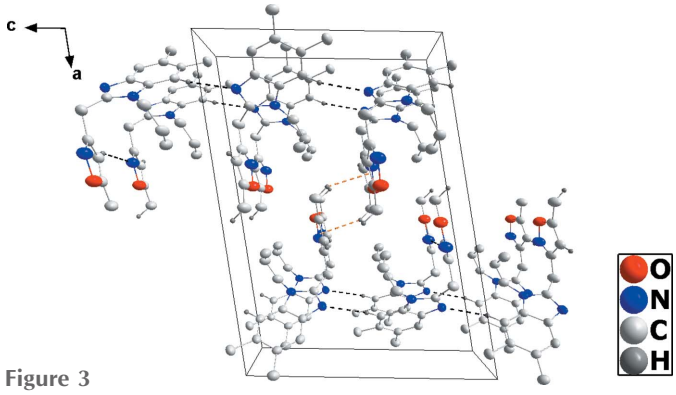

Figure 3
Packing viewed along the *b* axis (color code as in Fig. 2).

Tulane Crystallography Laboratory are gratefully acknowledged.

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full crystallographic data

IUCrData (2017). **2**, x170647 [https://doi.org/10.1107/S2414314617006472]

5,6-Dimethyl-2-[(5-methyl-1,2-oxazol-3-yl)methyl]-1-(prop-2-en-1-yl)-1*H*-1,3-benzodiazole

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Crystal data

$C_{17}H_{19}N_3O$
M_r = 281.35
Monoclinic, $P2_1/c$
a = 19.6067 (6) Å
b = 5.5438 (2) Å
c = 14.0069 (5) Å
β = 99.911 (2)°
V = 1499.77 (9) Å^3
Z = 4
$F(000)$ = 600
D_x = 1.246 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 5620 reflections
θ = 4.6–70.0°
μ = 0.63 mm^{-1}
T = 150 K
Plate, colourless
0.12 × 0.07 × 0.01 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.86, T_{max} = 0.99
10867 measured reflections
2825 independent reflections
2121 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 70.0°, θ_{min} = 2.3°
h = −23→23
k = −6→6
l = −15→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.111
S = 1.05
2825 reflections
267 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.5009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL 2014/7* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0045 (4)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.54770 (7)	1.1344 (3)	0.13741 (12)	0.0466 (4)
N1	0.80943 (8)	0.7372 (3)	0.15996 (11)	0.0339 (4)
N2	0.77640 (7)	0.9145 (3)	0.28924 (11)	0.0303 (4)
N3	0.61491 (9)	1.2309 (3)	0.13994 (14)	0.0457 (5)
C1	0.82047 (8)	0.7281 (3)	0.32548 (13)	0.0264 (4)
C2	0.84425 (8)	0.6479 (3)	0.41974 (13)	0.0275 (4)
H2	0.8297 (9)	0.725 (3)	0.4785 (14)	0.031 (5)*
C3	0.89030 (8)	0.4559 (3)	0.43144 (13)	0.0277 (4)
C4	0.91251 (8)	0.3476 (3)	0.35005 (13)	0.0283 (4)
C5	0.88754 (9)	0.4304 (4)	0.25751 (14)	0.0309 (4)
H5	0.9042 (11)	0.356 (4)	0.1992 (15)	0.040 (6)*
C6	0.84092 (8)	0.6209 (3)	0.24493 (13)	0.0285 (4)
C7	0.77223 (9)	0.9087 (4)	0.19014 (14)	0.0325 (4)
C8	0.91514 (10)	0.3569 (4)	0.53132 (14)	0.0356 (5)
H8A	0.9678 (11)	0.351 (4)	0.5505 (14)	0.039 (6)*
H8B	0.8968 (12)	0.454 (4)	0.5818 (17)	0.050 (6)*
H8C	0.8988 (11)	0.181 (4)	0.5357 (16)	0.048 (6)*
C9	0.96358 (10)	0.1413 (4)	0.36417 (17)	0.0378 (5)
H9A	0.9451 (12)	0.007 (5)	0.4013 (18)	0.058 (7)*
H9B	1.0101 (13)	0.191 (4)	0.4038 (17)	0.058 (7)*
H9C	0.9742 (12)	0.087 (4)	0.2990 (19)	0.061 (7)*
C10	0.72902 (10)	1.0819 (4)	0.12321 (17)	0.0409 (5)
H10A	0.7409 (11)	1.256 (4)	0.1425 (15)	0.045 (6)*
H10B	0.7401 (11)	1.053 (4)	0.0554 (17)	0.046 (6)*
C11	0.65309 (10)	1.0480 (3)	0.12356 (14)	0.0343 (5)
C12	0.61480 (10)	0.8321 (4)	0.11048 (14)	0.0343 (4)
H12	0.6306 (12)	0.664 (5)	0.0994 (17)	0.056 (7)*
C13	0.55011 (10)	0.8941 (4)	0.12044 (14)	0.0348 (4)
C14	0.48476 (11)	0.7599 (5)	0.1177 (2)	0.0465 (6)
H14A	0.4485 (14)	0.812 (5)	0.061 (2)	0.076 (9)*
H14B	0.4933 (15)	0.583 (6)	0.108 (2)	0.087 (10)*
H14C	0.4654 (13)	0.782 (5)	0.175 (2)	0.068 (8)*
C15	0.74467 (10)	1.0827 (4)	0.34788 (16)	0.0368 (5)
H15A	0.7314 (11)	1.234 (4)	0.3106 (17)	0.052 (6)*
H15B	0.7805 (11)	1.135 (4)	0.4056 (16)	0.046 (6)*

C16	0.68341 (10)	0.9834 (4)	0.38483 (16)	0.0414 (5)
H16	0.6641 (12)	1.081 (4)	0.4300 (17)	0.054 (7)*
C17	0.65382 (11)	0.7744 (5)	0.36319 (17)	0.0461 (6)
H17A	0.6126 (14)	0.723 (5)	0.3939 (19)	0.073 (8)*
H17B	0.6715 (11)	0.663 (4)	0.3190 (16)	0.046 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0367 (8)	0.0343 (8)	0.0677 (11)	0.0044 (6)	0.0064 (7)	0.0012 (7)
N1	0.0293 (8)	0.0430 (10)	0.0289 (9)	−0.0025 (7)	0.0032 (6)	0.0063 (7)
N2	0.0256 (7)	0.0284 (8)	0.0364 (9)	0.0005 (6)	0.0039 (6)	0.0036 (7)
N3	0.0377 (9)	0.0312 (9)	0.0657 (13)	−0.0019 (8)	0.0017 (8)	0.0037 (8)
C1	0.0208 (8)	0.0276 (9)	0.0300 (10)	−0.0014 (7)	0.0028 (7)	0.0019 (7)
C2	0.0236 (8)	0.0304 (10)	0.0287 (10)	−0.0034 (7)	0.0050 (7)	−0.0015 (8)
C3	0.0234 (8)	0.0324 (10)	0.0269 (10)	−0.0032 (7)	0.0030 (7)	0.0022 (7)
C4	0.0220 (8)	0.0302 (10)	0.0331 (10)	−0.0002 (7)	0.0056 (7)	−0.0012 (7)
C5	0.0272 (9)	0.0369 (11)	0.0297 (10)	−0.0013 (8)	0.0077 (7)	−0.0039 (8)
C6	0.0243 (8)	0.0357 (10)	0.0256 (9)	−0.0035 (8)	0.0046 (7)	0.0014 (8)
C7	0.0251 (8)	0.0374 (11)	0.0337 (11)	−0.0057 (8)	0.0013 (7)	0.0089 (8)
C8	0.0353 (10)	0.0403 (12)	0.0296 (11)	0.0023 (9)	0.0013 (8)	0.0044 (9)
C9	0.0307 (10)	0.0378 (12)	0.0445 (13)	0.0066 (9)	0.0053 (9)	−0.0009 (10)
C10	0.0320 (10)	0.0411 (13)	0.0471 (13)	−0.0024 (9)	−0.0001 (9)	0.0152 (10)
C11	0.0336 (9)	0.0298 (10)	0.0369 (11)	0.0020 (8)	−0.0013 (8)	0.0087 (8)
C12	0.0344 (10)	0.0294 (10)	0.0371 (11)	0.0008 (8)	0.0008 (8)	0.0028 (8)
C13	0.0345 (10)	0.0319 (11)	0.0361 (11)	−0.0004 (8)	0.0006 (8)	0.0039 (8)
C14	0.0336 (11)	0.0496 (15)	0.0549 (15)	−0.0051 (10)	0.0032 (10)	0.0080 (11)
C15	0.0316 (10)	0.0303 (11)	0.0468 (13)	0.0047 (8)	0.0022 (9)	−0.0039 (9)
C16	0.0305 (10)	0.0473 (13)	0.0460 (13)	0.0062 (10)	0.0053 (9)	−0.0081 (10)
C17	0.0355 (11)	0.0545 (15)	0.0496 (14)	−0.0031 (11)	0.0109 (10)	0.0001 (11)

Geometric parameters (Å, º)

O1—C13	1.356 (2)	C8—H8C	1.03 (2)
O1—N3	1.417 (2)	C9—H9A	1.01 (3)
N1—C7	1.312 (3)	C9—H9B	1.02 (3)
N1—C6	1.400 (2)	C9—H9C	1.02 (3)
N2—C7	1.377 (2)	C10—C11	1.501 (3)
N2—C1	1.386 (2)	C10—H10A	1.02 (2)
N2—C15	1.451 (2)	C10—H10B	1.02 (2)
N3—C11	1.304 (3)	C11—C12	1.408 (3)
C1—C6	1.394 (2)	C12—C13	1.344 (3)
C1—C2	1.395 (2)	C12—H12	1.00 (2)
C2—C3	1.387 (3)	C13—C14	1.476 (3)
C2—H2	1.010 (19)	C14—H14A	1.01 (3)
C3—C4	1.421 (2)	C14—H14B	1.01 (3)
C3—C8	1.504 (3)	C14—H14C	0.95 (3)
C4—C5	1.383 (3)	C15—C16	1.492 (3)

C4—C9	1.510 (3)	C15—H15A	1.00 (2)
C5—C6	1.388 (3)	C15—H15B	1.02 (2)
C5—H5	1.02 (2)	C16—C17	1.308 (3)
C7—C10	1.498 (3)	C16—H16	0.96 (2)
C8—H8A	1.02 (2)	C17—H17A	1.02 (3)
C8—H8B	1.00 (2)	C17—H17B	0.98 (2)

C13—O1—N3	108.37 (15)	C4—C9—H9C	109.9 (14)
C7—N1—C6	104.36 (15)	H9A—C9—H9C	113.1 (19)
C7—N2—C1	106.09 (15)	H9B—C9—H9C	105.5 (19)
C7—N2—C15	128.95 (16)	C7—C10—C11	111.83 (16)
C1—N2—C15	124.92 (16)	C7—C10—H10A	111.3 (12)
C11—N3—O1	105.15 (15)	C11—C10—H10A	107.5 (12)
N2—C1—C6	105.63 (15)	C7—C10—H10B	107.1 (12)
N2—C1—C2	132.06 (16)	C11—C10—H10B	110.7 (12)
C6—C1—C2	122.31 (16)	H10A—C10—H10B	108.5 (16)
C3—C2—C1	117.44 (16)	N3—C11—C12	112.00 (17)
C3—C2—H2	119.7 (11)	N3—C11—C10	120.16 (18)
C1—C2—H2	122.9 (11)	C12—C11—C10	127.81 (19)
C2—C3—C4	120.83 (16)	C13—C12—C11	105.13 (18)
C2—C3—C8	119.33 (17)	C13—C12—H12	125.1 (13)
C4—C3—C8	119.82 (17)	C11—C12—H12	129.7 (13)
C5—C4—C3	120.25 (16)	C12—C13—O1	109.34 (17)
C5—C4—C9	119.59 (17)	C12—C13—C14	134.3 (2)
C3—C4—C9	120.16 (17)	O1—C13—C14	116.33 (19)
C4—C5—C6	119.38 (17)	C13—C14—H14A	111.4 (15)
C4—C5—H5	120.4 (12)	C13—C14—H14B	109.3 (17)
C6—C5—H5	120.2 (12)	H14A—C14—H14B	107 (2)
C5—C6—C1	119.77 (16)	C13—C14—H14C	112.5 (16)
C5—C6—N1	129.98 (17)	H14A—C14—H14C	107 (2)
C1—C6—N1	110.23 (16)	H14B—C14—H14C	110 (2)
N1—C7—N2	113.69 (16)	N2—C15—C16	114.11 (17)
N1—C7—C10	123.28 (19)	N2—C15—H15A	110.0 (13)
N2—C7—C10	123.02 (19)	C16—C15—H15A	109.7 (13)
C3—C8—H8A	114.1 (12)	N2—C15—H15B	109.1 (12)
C3—C8—H8B	111.2 (13)	C16—C15—H15B	108.4 (12)
H8A—C8—H8B	107.5 (17)	H15A—C15—H15B	105.1 (18)
C3—C8—H8C	110.3 (12)	C17—C16—C15	126.7 (2)
H8A—C8—H8C	105.3 (17)	C17—C16—H16	116.4 (14)
H8B—C8—H8C	108.2 (17)	C15—C16—H16	116.9 (14)
C4—C9—H9A	109.7 (14)	C16—C17—H17A	120.1 (16)
C4—C9—H9B	112.0 (14)	C16—C17—H17B	121.0 (13)
H9A—C9—H9B	106.6 (19)	H17A—C17—H17B	119 (2)

C13—O1—N3—C11	0.7 (2)	C7—N1—C6—C1	0.6 (2)
C7—N2—C1—C6	0.45 (18)	C6—N1—C7—N2	−0.3 (2)
C15—N2—C1—C6	−177.34 (16)	C6—N1—C7—C10	179.90 (17)
C7—N2—C1—C2	179.60 (18)	C1—N2—C7—N1	−0.1 (2)

C15—N2—C1—C2	1.8 (3)	C15—N2—C7—N1	177.57 (17)
N2—C1—C2—C3	−178.43 (17)	C1—N2—C7—C10	179.71 (16)
C6—C1—C2—C3	0.6 (3)	C15—N2—C7—C10	−2.6 (3)
C1—C2—C3—C4	0.5 (2)	N1—C7—C10—C11	113.8 (2)
C1—C2—C3—C8	−177.59 (16)	N2—C7—C10—C11	−66.0 (3)
C2—C3—C4—C5	−1.0 (3)	O1—N3—C11—C12	−0.3 (2)
C8—C3—C4—C5	177.09 (17)	O1—N3—C11—C10	−178.57 (17)
C2—C3—C4—C9	178.99 (17)	C7—C10—C11—N3	126.8 (2)
C8—C3—C4—C9	−2.9 (3)	C7—C10—C11—C12	−51.2 (3)
C3—C4—C5—C6	0.3 (3)	N3—C11—C12—C13	−0.3 (2)
C9—C4—C5—C6	−179.63 (17)	C10—C11—C12—C13	177.8 (2)
C4—C5—C6—C1	0.7 (3)	C11—C12—C13—O1	0.8 (2)
C4—C5—C6—N1	179.09 (17)	C11—C12—C13—C14	−178.6 (2)
N2—C1—C6—C5	178.01 (15)	N3—O1—C13—C12	−1.0 (2)
C2—C1—C6—C5	−1.2 (3)	N3—O1—C13—C14	178.53 (18)
N2—C1—C6—N1	−0.65 (19)	C7—N2—C15—C16	104.1 (2)
C2—C1—C6—N1	−179.90 (16)	C1—N2—C15—C16	−78.7 (2)
C7—N1—C6—C5	−177.89 (19)	N2—C15—C16—C17	−5.9 (3)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the N3/O1/C11–C13 oxazole ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N1^{i}	1.010 (19)	2.65 (2)	3.603 (2)	157.9 (15)
C12—H12···N3^{ii}	1.00 (2)	2.50 (3)	3.358 (3)	143.6 (17)
C14—H14*A*···*Cg*1^{iii}	1.01 (3)	2.77 (3)	3.704 (3)	154 (2)

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