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3-Acetyl-1,5-diphenyl-1*H*-pyrazole-4-carbonitrile

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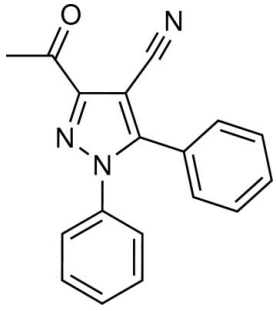
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.116; data-to-parameter ratio = 13.8.

The title compound, $C_{18}H_{13}N_3O$, has a butterfly-like structure, in which the pyrazole ring forms dihedral angles of 59.31 (8) and 57.24 (8)° with the two phenyl rings. The dihedral angle between the two phenyl rings is 64.03 (8)°. The pyrazole ring and the C—C═O plane of the acetyl group are twisted slightly, making a dihedral angle of 7.95 (18)°. In the crystal, molecules are linked through weak C—H···N and C—H···O interactions into a helical chain along the *a*-axis direction.

Related literature

For bond-length data, see: Allen *et al.* (1987). For background to and the bioactivity of pyrazole derivatives, see: Abdel-Aziz *et al.* (2009, 2010); Abdel-Wahab *et al.* (2009); Bharate *et al.* (2008); Dawood *et al.* (2003); Fu *et al.* (2010); Thumar & Patel (2011). For a related structure, see: Abdel-Aziz *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{13}N_3O$
M_r = 287.31
Orthorhombic, *Pbca*
a = 6.8322 (2) Å
b = 16.8974 (5) Å
c = 25.7968 (6) Å
V = 2978.15 (14) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.66 mm^{-1}
T = 296 K
0.56 × 0.35 × 0.23 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.708, T_{max} = 0.863
10678 measured reflections
2782 independent reflections
2338 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.08
2782 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6A···N3^{i}	0.93	2.53	3.432 (2)	165
C16—H16A···O1^{ii}	0.93	2.59	3.3758 (19)	142

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5091).

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supporting information

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3-Acetyl-1,5-diphenyl-1*H*-pyrazole-4-carbonitrile

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S1. Comment

Owing to the various biological properties of pyrazole derivatives such as anti-cancer (Fu *et al.*, 2010), anti-inflammatory (Bharate *et al.*, 2008) and antimicrobial activities (Thumar & Patel, 2011), we have during the course of our medicinal chemistry research reported the synthesis and bioactivity of pyrazole derivatives (Abdel-Aziz *et al.*, 2009, 2010; Abdel-Wahab *et al.*, 2009). The title compound (I) was synthesized and characterized in order to study the structure activity relationship of this class of compounds.

The molecule of (I), $C_{18}H_{13}N_3O$, has a butterfly-like structure. The pyrazole ring forms the dihedral angles of 59.31 (8) and 57.24 (8)°, respectively, with the C5–C10 and C11–C16 phenyl rings, whereas the dihedral angle between these two rings is 64.03 (8)°. The cabonitrile substituent lies on the same plane with the pyrazole ring with an *r.m.s*. 0.0027 (1) Å for the seven non-H atoms (C1–C4/N1–N3), whereas the acetyl group is slightly deviated with the torsion angles N2–C1–C17–C18 = 8.3 (2)° and N2–C1–C17–O1 = -171.47 (13)°. The bond distances in (I) are within normal ranges (Allen *et al.*, 1987) and comparable to the related structure (Abdel-Aziz *et al.*, 2011). The crystal packing of (I) is stabilized by weak C—H···N and C—H···O interactions (Table 1). Figure 2 shows the molecular a helical chain along the [1 0 0] linked by these interactions.

S2. Experimental

The title compound was prepared according to the reported method (Dawood *et al.*, 2003). Single crystals of the title compound suitable for X-ray structure determination were recrystallized from ethanol by the slow evaporation of the solvent at room temperature after several days.

S3. Refinement

All H atoms were placed in calculated positions with d(C—H) = 0.93 for aromatic and 0.96 Å for CH_3 atoms. The U_{iso}(H) 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.

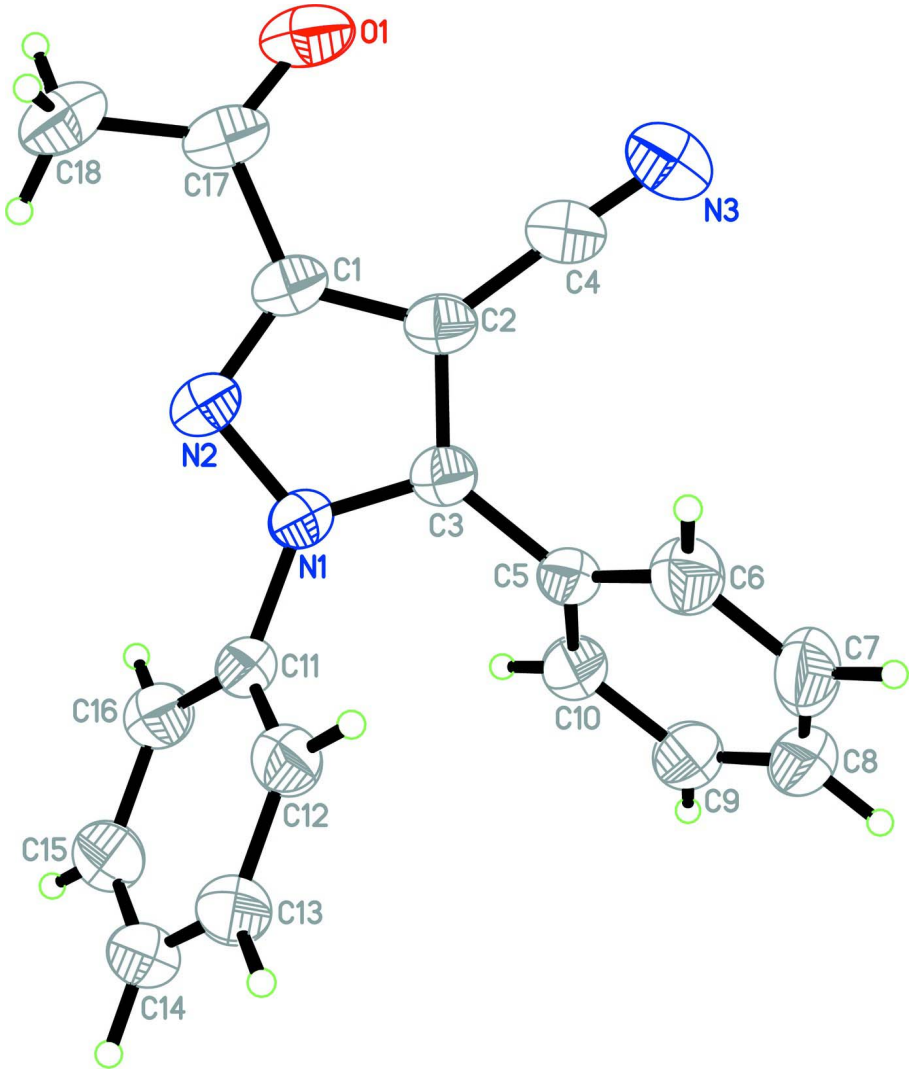

Figure 1

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

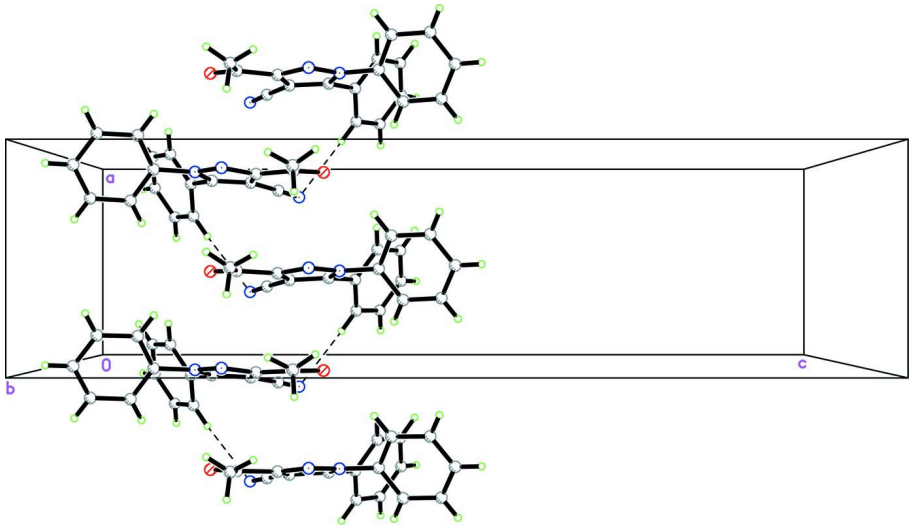

Figure 2

The crystal packing diagram of the title compound viewed along the *b* axis, showing the helical chain along the [1 0 0]. C—H···N hydrogen bonds are shown as dashed lines.

3-Acetyl-1,5-diphenyl-1*H*-pyrazole-4-carbonitrile

Crystal data

$C_{18}H_{13}N_3O$
$M_r = 287.31$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 6.8322\ (2)$ Å
$b = 16.8974\ (5)$ Å
$c = 25.7968\ (6)$ Å
$V = 2978.15\ (14)$ Å^3
$Z = 8$
$F(000) = 1200$
$D_x = 1.282$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 2782 reflections
$\theta = 3.4$–$69.9°$
$\mu = 0.66$ mm^{-1}
$T = 296$ K
Block, colorless
0.56 × 0.35 × 0.23 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.708$, $T_{max} = 0.863$
10678 measured reflections
2782 independent reflections
2338 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 69.9°$, $\theta_{min} = 3.4°$
$h = -6 \rightarrow 8$
$k = -20 \rightarrow 20$
$l = -31 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.116$
$S = 1.08$
2782 reflections
201 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 0.4109P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0012 (2)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.04907 (16)	0.77988 (6)	0.34667 (4)	0.0461 (3)
N2	0.03430 (17)	0.83315 (7)	0.30758 (4)	0.0501 (3)
N3	0.1596 (2)	0.59304 (10)	0.21580 (6)	0.0737 (4)
O1	0.05198 (19)	0.78631 (8)	0.17444 (4)	0.0747 (4)
C1	0.06117 (18)	0.79131 (8)	0.26452 (5)	0.0480 (3)
C2	0.09573 (19)	0.71052 (8)	0.27627 (5)	0.0463 (3)
C3	0.08526 (18)	0.70532 (8)	0.32961 (5)	0.0441 (3)
C4	0.1299 (2)	0.64619 (10)	0.24210 (5)	0.0536 (4)
C5	0.0947 (2)	0.63535 (8)	0.36354 (5)	0.0458 (3)
C6	0.2582 (2)	0.58729 (10)	0.36412 (6)	0.0628 (4)
H6A	0.3661	0.5995	0.3436	0.075*
C7	0.2603 (3)	0.52048 (10)	0.39553 (8)	0.0783 (5)
H7A	0.3702	0.4880	0.3961	0.094*
C8	0.1016 (4)	0.50213 (10)	0.42561 (7)	0.0785 (6)
H8A	0.1043	0.4575	0.4467	0.094*
C9	−0.0597 (3)	0.54911 (10)	0.42477 (7)	0.0741 (5)
H9A	−0.1675	0.5363	0.4451	0.089*
C10	−0.0647 (2)	0.61553 (9)	0.39400 (6)	0.0580 (4)
H10A	−0.1758	0.6473	0.3937	0.070*
C11	0.0388 (2)	0.80605 (8)	0.39950 (5)	0.0466 (3)
C12	0.1957 (2)	0.79135 (9)	0.43180 (6)	0.0566 (4)
H12A	0.3064	0.7656	0.4194	0.068*
C13	0.1858 (3)	0.81549 (10)	0.48280 (6)	0.0650 (4)
H13A	0.2901	0.8055	0.5050	0.078*
C14	0.0225 (3)	0.85426 (9)	0.50097 (6)	0.0658 (4)
H14A	0.0164	0.8703	0.5354	0.079*
C15	−0.1319 (3)	0.86926 (10)	0.46807 (6)	0.0662 (4)
H15A	−0.2414	0.8961	0.4803	0.079*
C16	−0.1254 (2)	0.84480 (9)	0.41697 (6)	0.0576 (4)
H16A	−0.2302	0.8544	0.3948	0.069*
C17	0.0492 (2)	0.82851 (10)	0.21251 (5)	0.0568 (4)
C18	0.0336 (3)	0.91591 (11)	0.20952 (7)	0.0755 (5)

H18A	−0.0431	0.9303	0.1798	0.113*
H18C	0.1621	0.9384	0.2065	0.113*
H18D	−0.0284	0.9356	0.2403	0.113*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0550 (6)	0.0450 (6)	0.0383 (5)	−0.0011 (5)	−0.0011 (4)	0.0056 (4)
N2	0.0541 (6)	0.0525 (6)	0.0438 (6)	−0.0019 (5)	−0.0021 (5)	0.0112 (5)
N3	0.0732 (9)	0.0852 (10)	0.0626 (8)	0.0025 (8)	0.0026 (7)	−0.0182 (8)
O1	0.0859 (8)	0.0965 (9)	0.0417 (6)	−0.0136 (7)	−0.0014 (5)	0.0109 (6)
C1	0.0429 (6)	0.0603 (8)	0.0407 (7)	−0.0073 (6)	−0.0012 (5)	0.0096 (6)
C2	0.0429 (6)	0.0566 (8)	0.0395 (6)	−0.0071 (6)	0.0003 (5)	0.0014 (6)
C3	0.0446 (6)	0.0474 (7)	0.0404 (6)	−0.0036 (5)	0.0002 (5)	0.0014 (5)
C4	0.0479 (7)	0.0701 (9)	0.0429 (7)	−0.0050 (7)	0.0009 (6)	−0.0026 (7)
C5	0.0579 (7)	0.0430 (7)	0.0363 (6)	−0.0014 (6)	−0.0021 (5)	−0.0020 (5)
C6	0.0642 (9)	0.0621 (9)	0.0622 (9)	0.0079 (7)	−0.0024 (7)	−0.0025 (7)
C7	0.0960 (13)	0.0558 (9)	0.0832 (12)	0.0250 (9)	−0.0237 (11)	−0.0051 (9)
C8	0.1315 (17)	0.0486 (9)	0.0554 (9)	0.0027 (10)	−0.0064 (10)	0.0067 (7)
C9	0.1125 (14)	0.0530 (9)	0.0568 (9)	−0.0034 (9)	0.0177 (9)	0.0085 (7)
C10	0.0738 (9)	0.0493 (8)	0.0508 (8)	0.0007 (7)	0.0113 (7)	0.0040 (6)
C11	0.0603 (7)	0.0395 (6)	0.0400 (6)	−0.0025 (6)	−0.0011 (6)	0.0034 (5)
C12	0.0651 (9)	0.0520 (8)	0.0526 (8)	0.0055 (7)	−0.0077 (6)	−0.0043 (6)
C13	0.0863 (11)	0.0575 (9)	0.0511 (8)	0.0016 (8)	−0.0186 (8)	−0.0037 (7)
C14	0.0962 (12)	0.0568 (9)	0.0445 (8)	−0.0048 (8)	−0.0002 (8)	−0.0051 (7)
C15	0.0801 (10)	0.0616 (9)	0.0571 (9)	0.0084 (8)	0.0100 (8)	−0.0040 (7)
C16	0.0650 (9)	0.0580 (8)	0.0499 (8)	0.0069 (7)	−0.0005 (6)	0.0038 (7)
C17	0.0460 (7)	0.0792 (10)	0.0451 (8)	−0.0084 (7)	−0.0012 (6)	0.0152 (7)
C18	0.0816 (11)	0.0821 (12)	0.0627 (10)	0.0030 (9)	0.0005 (8)	0.0291 (9)

Geometric parameters (Å, º)

N1—N2	1.3555 (15)	C9—C10	1.375 (2)
N1—C3	1.3572 (17)	C9—H9A	0.9300
N1—C11	1.4346 (17)	C10—H10A	0.9300
N2—C1	1.3294 (18)	C11—C16	1.375 (2)
N3—C4	1.144 (2)	C11—C12	1.380 (2)
O1—C17	1.214 (2)	C12—C13	1.379 (2)
C1—C2	1.418 (2)	C12—H12A	0.9300
C1—C17	1.4840 (18)	C13—C14	1.376 (3)
C2—C3	1.3807 (18)	C13—H13A	0.9300
C2—C4	1.419 (2)	C14—C15	1.378 (2)
C3—C5	1.4724 (18)	C14—H14A	0.9300
C5—C6	1.381 (2)	C15—C16	1.382 (2)
C5—C10	1.384 (2)	C15—H15A	0.9300
C6—C7	1.390 (2)	C16—H16A	0.9300
C6—H6A	0.9300	C17—C18	1.483 (2)
C7—C8	1.369 (3)	C18—H18A	0.9600

C7—H7A	0.9300	C18—H18C	0.9600
C8—C9	1.359 (3)	C18—H18D	0.9600
C8—H8A	0.9300		

N2—N1—C3	112.88 (11)	C9—C10—H10A	119.8
N2—N1—C11	119.90 (10)	C5—C10—H10A	119.8
C3—N1—C11	127.08 (11)	C16—C11—C12	121.44 (13)
C1—N2—N1	104.96 (11)	C16—C11—N1	119.87 (12)
N2—C1—C2	110.88 (11)	C12—C11—N1	118.69 (12)
N2—C1—C17	121.50 (13)	C13—C12—C11	118.99 (15)
C2—C1—C17	127.60 (13)	C13—C12—H12A	120.5
C3—C2—C1	105.40 (12)	C11—C12—H12A	120.5
C3—C2—C4	125.39 (13)	C14—C13—C12	120.36 (15)
C1—C2—C4	129.20 (13)	C14—C13—H13A	119.8
N1—C3—C2	105.88 (11)	C12—C13—H13A	119.8
N1—C3—C5	124.11 (11)	C13—C14—C15	119.91 (14)
C2—C3—C5	129.87 (12)	C13—C14—H14A	120.0
N3—C4—C2	177.90 (16)	C15—C14—H14A	120.0
C6—C5—C10	119.21 (14)	C14—C15—C16	120.54 (15)
C6—C5—C3	120.93 (13)	C14—C15—H15A	119.7
C10—C5—C3	119.83 (12)	C16—C15—H15A	119.7
C5—C6—C7	119.48 (16)	C11—C16—C15	118.75 (15)
C5—C6—H6A	120.3	C11—C16—H16A	120.6
C7—C6—H6A	120.3	C15—C16—H16A	120.6
C8—C7—C6	120.43 (17)	O1—C17—C18	122.97 (14)
C8—C7—H7A	119.8	O1—C17—C1	118.81 (15)
C6—C7—H7A	119.8	C18—C17—C1	118.22 (14)
C9—C8—C7	120.07 (16)	C17—C18—H18A	109.5
C9—C8—H8A	120.0	C17—C18—H18C	109.5
C7—C8—H8A	120.0	H18A—C18—H18C	109.5
C8—C9—C10	120.41 (18)	C17—C18—H18D	109.5
C8—C9—H9A	119.8	H18A—C18—H18D	109.5
C10—C9—H9A	119.8	H18C—C18—H18D	109.5
C9—C10—C5	120.39 (16)		

C3—N1—N2—C1	0.20 (14)	C5—C6—C7—C8	0.2 (3)
C11—N1—N2—C1	176.31 (11)	C6—C7—C8—C9	0.3 (3)
N1—N2—C1—C2	−0.67 (14)	C7—C8—C9—C10	−0.4 (3)
N1—N2—C1—C17	177.93 (11)	C8—C9—C10—C5	0.0 (3)
N2—C1—C2—C3	0.89 (15)	C6—C5—C10—C9	0.5 (2)
C17—C1—C2—C3	−177.61 (12)	C3—C5—C10—C9	178.21 (14)
N2—C1—C2—C4	179.54 (13)	N2—N1—C11—C16	59.51 (17)
C17—C1—C2—C4	1.0 (2)	C3—N1—C11—C16	−124.99 (15)
N2—N1—C3—C2	0.34 (14)	N2—N1—C11—C12	−120.59 (14)
C11—N1—C3—C2	−175.42 (12)	C3—N1—C11—C12	54.91 (19)
N2—N1—C3—C5	−175.66 (11)	C16—C11—C12—C13	0.7 (2)
C11—N1—C3—C5	8.6 (2)	N1—C11—C12—C13	−179.21 (13)
C1—C2—C3—N1	−0.71 (14)	C11—C12—C13—C14	−0.6 (2)

C4—C2—C3—N1	−179.43 (12)	C12—C13—C14—C15	−0.1 (3)
C1—C2—C3—C5	174.97 (13)	C13—C14—C15—C16	0.8 (3)
C4—C2—C3—C5	−3.7 (2)	C12—C11—C16—C15	0.0 (2)
N1—C3—C5—C6	−124.42 (15)	N1—C11—C16—C15	179.86 (14)
C2—C3—C5—C6	60.6 (2)	C14—C15—C16—C11	−0.7 (3)
N1—C3—C5—C10	57.90 (18)	N2—C1—C17—O1	−171.47 (13)
C2—C3—C5—C10	−117.09 (16)	C2—C1—C17—O1	6.9 (2)
C10—C5—C6—C7	−0.5 (2)	N2—C1—C17—C18	8.3 (2)
C3—C5—C6—C7	−178.24 (14)	C2—C1—C17—C18	−173.32 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···N3^{i}	0.93	2.53	3.432 (2)	165
C16—H16*A*···O1^{ii}	0.93	2.59	3.3758 (19)	142

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