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2-(1*H*-indol-3-ylcarbonyl)acetonitrile

P. Ramesh,[a] A. Subbiahpandi,[a] P. Thirumurugan,[b] Paramasivan T. Perumal[b] and M. N. Ponnuswamy[c]*

[a]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India, [b]Organic Chemistry Division, Central Leather Research Institute, Adyar, Chennai 600 020, India, and [c]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India
Correspondence e-mail: mnpsy2004@yahoo.com

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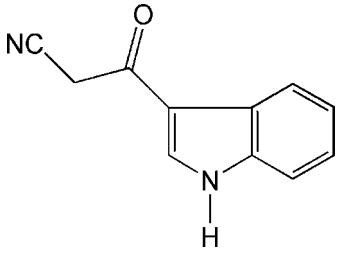
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.100; data-to-parameter ratio = 12.9.

The title compound, $C_{11}H_8N_2O$, crystallizes with two crystallographically independent molecules in the asymmetric unit which are approximately perpendicular to each other [79.97 (6)°]. The indole ring system is planar [r.m.s. deviation = 0.010 (1) Å]. The crystal structure is stabilized by intermolecular C—H···N and N—H···O interactions.

Related literature

For the use of indole derivatives as bioactive drugs, see: Stevenson *et al.* (2000). For their biological properties, see: Harris & Uhle (1960); Ho *et al.* (1986). For their high aldose reductase inhibitory activity, see: Rajeswaran *et al.* (1999). For a related structure, see: Ramesh *et al.* (2008). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{11}H_8N_2O$
M_r = 184.19
Triclinic, $P\overline{1}$
a = 7.3439 (2) Å
b = 7.3534 (2) Å
c = 18.2475 (5) Å
α = 83.402 (2)°
β = 78.890 (2)°
γ = 73.501 (1)°
V = 925.23 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker Kappa APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.974, T_{max} = 0.983
18838 measured reflections
3253 independent reflections
2717 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.06
3253 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 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—H1···O1^{i}	0.86	1.98	2.8146 (18)	163
C2—H2···N13^{i}	0.93	2.59	3.236 (2)	127
N1′—H1′···O1′^{ii}	0.86	2.00	2.8166 (15)	158

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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* and *PLATON* (Spek, 2003).

PR thanks Dr Babu Varghese, SAIF, IIT-Madras, India, for his help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2839).

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2-(1*H*-indol-3-ylcarbonyl)acetonitrile

P. Ramesh, A. Subbiahpandi, P. Thirumurugan, Paramasivan T. Perumal and M. N. Ponnuswamy

S1. Comment

Indole derivatives are used as bioactive drugs (Stevenson *et al.*, 2000) and they exibit anti-allergic, central nervous system depressant and muscle relaxant properties (Harris & Uhle 1960; Ho *et al.*, 1986). Indoles have been proved to display high aldose reductase inhibitory activity (Rajeswaran *et al.*, 1999). Against this background and to ascertain the molecular conformation, the structure determination of the title compound has been carried out.

There are two crystallographically independent molecules in the asymmetric unit and they are approximately perpendicular to each other [79.97 (6)°]. In both molecules the indole ring systems are planar and the sum of the angles at N1 (359.95°) and N1′ (359.94°) are in accordance with sp^2 hybridization. The bond angles of the cyano group [179.8 (2) and 179.6 (2)°] in both molecules show their linear character. The C≡N bond distances [1.133 (2) and 1.131 (2) Å] are comparable with the literature values (Ramesh *et al.*, 2008).

The crystal packing is covered by C—H···N, C—H···O and C—H···π types intermolecular interactions in addition to van der Waals forces. N1 atom in one of the molecules donates one proton to O1 (-1 + *x*, *y*, *z*) which connects the molecules into a one dimensional C6 chain (Bernstein *et al.*, 1995) running along the *a* axis, whereas in the other molecule at N1′ forms similar network with O1′ (*x*, 1 + *y*, *z*) along the *b* axis. The combination of N1—H1···O1 and C2—H2···N13 hydrogen bonds form a R_2^2 (9) dimer chain running along the *a* axis.

S2. Experimental

Indole (5.85 g, 50 mmol) was added to a solution prepared by dissolution of cyanoacetic acid (5.0 g, 50 mmol) in Ac_2O (50 ml) at 50 °C. The solution was heated at 85 °C for 5 min. During that period 3-cyanoacetylindole started to crystallize. After 5 more min, the mixture was allowed to cool and the solid was collected, washed with MeOH, and dried.

S3. Refinement

H atoms were positioned geometrically (N—H = 0.86 Å, and C—H = 0.93–0.97 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H, 1.2U_{eq}(C) for other H atoms.

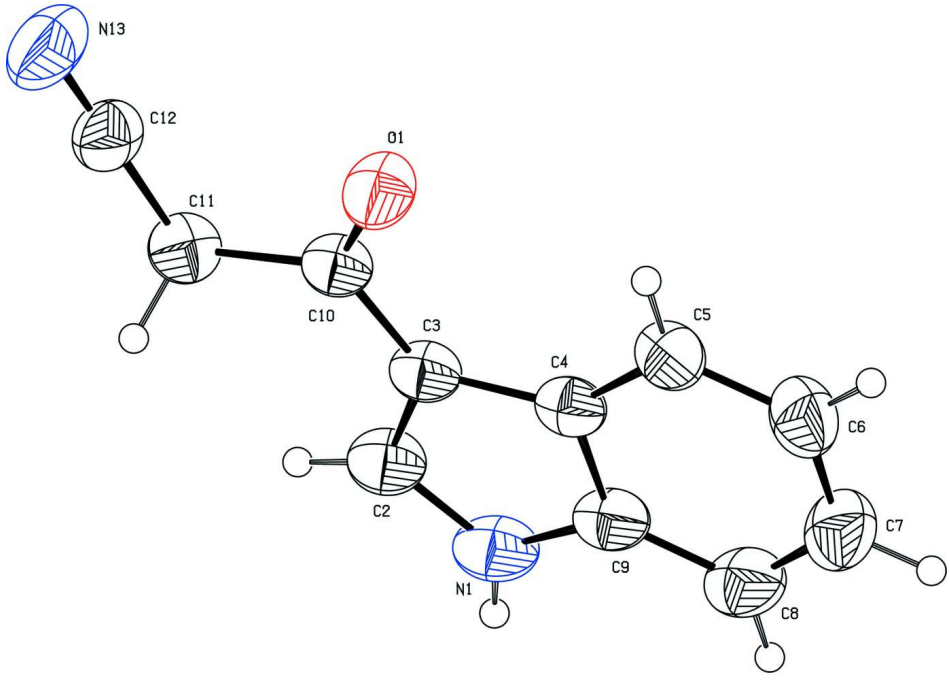

Figure 1

Perspective view of the molecule showing the thermal ellipsoids are drawn at 50% probability level. The H atoms are shown as small circles of arbitrary radii.

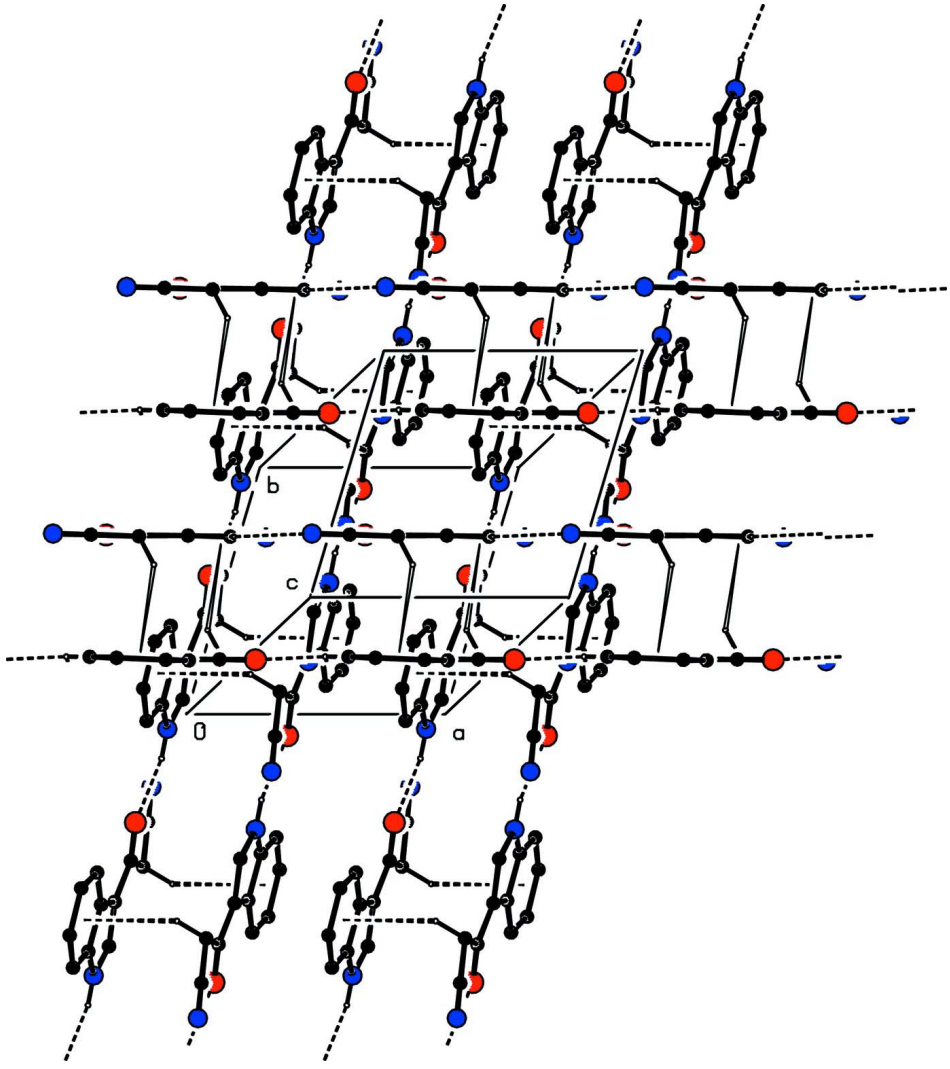

Figure 2

The crystal packing of the molecules viewed down *c* axis. H atoms not involved in hydrogen bonding have been omitted for clarity.

2-(1*H*-indol-3-ylcarbonyl)acetonitrile

Crystal data

$C_{11}H_8N_2O$
$M_r = 184.19$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.3439\ (2)$ Å
$b = 7.3534\ (2)$ Å
$c = 18.2475\ (5)$ Å
$\alpha = 83.402\ (2)°$
$\beta = 78.890\ (2)°$
$\gamma = 73.501\ (1)°$
$V = 925.23\ (4)$ Å^3
$Z = 4$
$F(000) = 384$
$D_x = 1.322$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3554 reflections
$\theta = 1.1–25.0°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker Kappa APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.974, T_{max} = 0.983
18838 measured reflections
3253 independent reflections
2717 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°, θ_{min} = 1.1°
$h = -7 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.06
3253 reflections
253 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
$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.2437P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.008
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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}
O1	0.13478 (16)	0.2464 (2)	1.01403 (7)	0.0659 (4)
O1′	0.76317 (17)	0.33368 (14)	0.47980 (6)	0.0543 (3)
N1	0.7573 (2)	0.2397 (2)	1.00692 (9)	0.0619 (4)
H1	0.8678	0.2314	1.0183	0.074*
N1′	0.77718 (19)	−0.28849 (17)	0.48288 (7)	0.0479 (3)
H1′	0.7932	−0.4024	0.4709	0.057*
C2	0.6023 (2)	0.2202 (2)	1.05570 (11)	0.0567 (4)
H2	0.5977	0.1956	1.1071	0.068*
C2′	0.8188 (2)	−0.1468 (2)	0.43593 (9)	0.0441 (4)
H2′	0.8689	−0.1567	0.3853	0.053*
C3	0.4501 (2)	0.2418 (2)	1.01850 (9)	0.0475 (4)
C3′	0.7768 (2)	0.01550 (19)	0.47349 (8)	0.0385 (3)
C4	0.5195 (2)	0.2786 (2)	0.94094 (9)	0.0478 (4)
C4′	0.7012 (2)	−0.03211 (19)	0.54959 (8)	0.0389 (3)
C5′	0.6267 (2)	0.0675 (2)	0.61400 (9)	0.0479 (4)
H5′	0.6214	0.1956	0.6133	0.058*

C5	0.4391 (2)	0.3141 (2)	0.87583 (10)	0.0565 (4)
H5	0.3107	0.3175	0.8777	0.068*
C6′	0.5613 (3)	−0.0269 (2)	0.67853 (9)	0.0569 (4)
H6′	0.5098	0.0389	0.7216	0.068*
C6	0.5521 (3)	0.3437 (3)	0.80899 (11)	0.0678 (5)
H6	0.4991	0.3687	0.7653	0.081*
C7′	0.5702 (3)	−0.2187 (2)	0.68090 (10)	0.0583 (4)
H7′	0.5269	−0.2792	0.7257	0.070*
C7	0.7456 (3)	0.3370 (3)	0.80531 (13)	0.0742 (6)
H7	0.8195	0.3559	0.7591	0.089*
C8′	0.6417 (2)	−0.3200 (2)	0.61849 (10)	0.0527 (4)
H8′	0.6475	−0.4483	0.6199	0.063*
C8	0.8287 (3)	0.3032 (3)	0.86844 (13)	0.0684 (5)
H8	0.9574	0.2993	0.8660	0.082*
C9	0.7140 (2)	0.2751 (2)	0.93550 (11)	0.0540 (4)
C9′	0.7049 (2)	−0.2241 (2)	0.55332 (8)	0.0419 (3)
C10	0.2612 (2)	0.2273 (2)	1.05110 (9)	0.0482 (4)
C10′	0.8024 (2)	0.19645 (19)	0.44251 (8)	0.0396 (3)
C11′	0.8851 (2)	0.2118 (2)	0.35992 (8)	0.0455 (4)
H11A	1.0210	0.1451	0.3524	0.055*
H11B	0.8214	0.1505	0.3322	0.055*
C11	0.2210 (2)	0.1842 (3)	1.13506 (9)	0.0562 (4)
H11C	0.3072	0.0628	1.1480	0.067*
H11D	0.2474	0.2809	1.1602	0.067*
C12	0.0245 (3)	0.1779 (3)	1.16141 (9)	0.0605 (5)
C12′	0.8620 (2)	0.4067 (2)	0.33086 (9)	0.0513 (4)
N13	−0.1297 (3)	0.1725 (3)	1.18193 (9)	0.0878 (6)
N13′	0.8429 (3)	0.5597 (2)	0.30820 (9)	0.0806 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0436 (6)	0.1027 (10)	0.0585 (7)	−0.0291 (6)	−0.0166 (6)	0.0039 (7)
O1′	0.0829 (8)	0.0340 (6)	0.0491 (6)	−0.0248 (5)	−0.0035 (6)	−0.0054 (5)
N1	0.0409 (8)	0.0647 (9)	0.0868 (11)	−0.0155 (7)	−0.0217 (8)	−0.0100 (8)
N1′	0.0611 (8)	0.0298 (6)	0.0566 (8)	−0.0163 (6)	−0.0112 (6)	−0.0059 (6)
C2	0.0469 (9)	0.0597 (10)	0.0689 (11)	−0.0150 (8)	−0.0187 (8)	−0.0087 (8)
C2′	0.0521 (9)	0.0379 (8)	0.0453 (8)	−0.0158 (6)	−0.0082 (7)	−0.0056 (6)
C3	0.0412 (8)	0.0451 (9)	0.0602 (10)	−0.0126 (7)	−0.0144 (7)	−0.0072 (7)
C3′	0.0432 (8)	0.0323 (7)	0.0435 (8)	−0.0136 (6)	−0.0109 (6)	−0.0027 (6)
C4	0.0420 (8)	0.0367 (8)	0.0674 (11)	−0.0124 (6)	−0.0128 (7)	−0.0038 (7)
C4′	0.0409 (8)	0.0333 (7)	0.0461 (8)	−0.0130 (6)	−0.0123 (6)	−0.0011 (6)
C5′	0.0566 (9)	0.0388 (8)	0.0501 (9)	−0.0144 (7)	−0.0095 (7)	−0.0043 (7)
C5	0.0509 (9)	0.0527 (10)	0.0689 (11)	−0.0184 (8)	−0.0160 (8)	0.0048 (8)
C6′	0.0671 (11)	0.0573 (10)	0.0458 (9)	−0.0172 (8)	−0.0067 (8)	−0.0043 (8)
C6	0.0761 (13)	0.0590 (11)	0.0706 (13)	−0.0260 (9)	−0.0147 (10)	0.0103 (9)
C7′	0.0656 (11)	0.0587 (11)	0.0514 (10)	−0.0237 (8)	−0.0092 (8)	0.0103 (8)
C7	0.0741 (13)	0.0641 (12)	0.0810 (14)	−0.0287 (10)	0.0052 (11)	0.0041 (10)

C8′	0.0611 (10)	0.0385 (8)	0.0623 (11)	−0.0213 (7)	−0.0151 (8)	0.0093 (7)
C8	0.0486 (10)	0.0584 (11)	0.0983 (16)	−0.0215 (8)	−0.0032 (10)	−0.0021 (10)
C9	0.0424 (9)	0.0429 (9)	0.0794 (12)	−0.0144 (7)	−0.0114 (8)	−0.0055 (8)
C9′	0.0443 (8)	0.0348 (7)	0.0498 (9)	−0.0136 (6)	−0.0119 (7)	−0.0016 (6)
C10	0.0438 (8)	0.0472 (9)	0.0576 (10)	−0.0131 (7)	−0.0148 (7)	−0.0065 (7)
C10′	0.0432 (8)	0.0347 (7)	0.0446 (8)	−0.0140 (6)	−0.0106 (6)	−0.0026 (6)
C11′	0.0512 (9)	0.0421 (8)	0.0451 (9)	−0.0155 (7)	−0.0081 (7)	−0.0026 (7)
C11	0.0554 (10)	0.0621 (10)	0.0551 (10)	−0.0163 (8)	−0.0154 (8)	−0.0085 (8)
C12	0.0591 (12)	0.0765 (12)	0.0430 (9)	−0.0117 (9)	−0.0078 (8)	−0.0100 (8)
C12′	0.0641 (10)	0.0487 (10)	0.0432 (9)	−0.0227 (8)	−0.0044 (8)	0.0001 (7)
N13	0.0640 (11)	0.1429 (18)	0.0513 (10)	−0.0231 (11)	−0.0009 (8)	−0.0111 (10)
N13′	0.1215 (15)	0.0564 (10)	0.0620 (10)	−0.0331 (10)	−0.0029 (10)	0.0065 (8)

Geometric parameters (Å, º)

O1—C10	1.2190 (18)	C5—H5	0.9300
O1′—C10′	1.2173 (17)	C6′—C7′	1.389 (2)
N1—C2	1.335 (2)	C6′—H6′	0.9300
N1—C9	1.379 (2)	C6—C7	1.396 (3)
N1—H1	0.8600	C6—H6	0.9300
N1′—C2′	1.3372 (19)	C7′—C8′	1.367 (2)
N1′—C9′	1.3755 (19)	C7′—H7′	0.9300
N1′—H1′	0.8600	C7—C8	1.371 (3)
C2—C3	1.379 (2)	C7—H7	0.9300
C2—H2	0.9300	C8′—C9′	1.381 (2)
C2′—C3′	1.373 (2)	C8′—H8′	0.9300
C2′—H2′	0.9300	C8—C9	1.376 (3)
C3—C10	1.429 (2)	C8—H8	0.9300
C3—C4	1.431 (2)	C10—C11	1.517 (2)
C3′—C10′	1.4331 (19)	C10′—C11′	1.516 (2)
C3′—C4′	1.436 (2)	C11′—C12′	1.445 (2)
C4—C5	1.393 (2)	C11′—H11A	0.9700
C4—C9	1.406 (2)	C11′—H11B	0.9700
C4′—C5′	1.393 (2)	C11—C12	1.443 (3)
C4′—C9′	1.3987 (19)	C11—H11C	0.9700
C5′—C6′	1.372 (2)	C11—H11D	0.9700
C5′—H5′	0.9300	C12—N13	1.133 (2)
C5—C6	1.369 (3)	C12′—N13′	1.132 (2)
C2—N1—C9	109.94 (14)	C8′—C7′—H7′	119.4
C2—N1—H1	125.0	C6′—C7′—H7′	119.4
C9—N1—H1	125.0	C8—C7—C6	121.35 (19)
C2′—N1′—C9′	109.56 (12)	C8—C7—H7	119.3
C2′—N1′—H1′	125.2	C6—C7—H7	119.3
C9′—N1′—H1′	125.2	C7′—C8′—C9′	117.34 (15)
N1—C2—C3	109.81 (16)	C7′—C8′—H8′	121.3
N1—C2—H2	125.1	C9′—C8′—H8′	121.3
C3—C2—H2	125.1	C7—C8—C9	117.29 (18)

N1′—C2′—C3′	110.07 (14)	C7—C8—H8	121.4
N1′—C2′—H2′	125.0	C9—C8—H8	121.4
C3′—C2′—H2′	125.0	C8—C9—N1	130.03 (16)
C2—C3—C10	126.55 (16)	C8—C9—C4	122.72 (17)
C2—C3—C4	106.56 (14)	N1—C9—C4	107.25 (15)
C10—C3—C4	126.89 (14)	N1′—C9′—C8′	129.55 (14)
C2′—C3′—C10′	126.66 (14)	N1′—C9′—C4′	107.66 (13)
C2′—C3′—C4′	106.34 (12)	C8′—C9′—C4′	122.78 (14)
C10′—C3′—C4′	126.99 (13)	O1—C10—C3	122.51 (15)
C5—C4—C9	118.60 (16)	O1—C10—C11	119.87 (15)
C5—C4—C3	134.95 (15)	C3—C10—C11	117.61 (13)
C9—C4—C3	106.45 (14)	O1′—C10′—C3′	122.74 (13)
C5′—C4′—C9′	118.54 (13)	O1′—C10′—C11′	120.06 (13)
C5′—C4′—C3′	135.07 (13)	C3′—C10′—C11′	117.20 (12)
C9′—C4′—C3′	106.36 (12)	C12′—C11′—C10′	112.33 (13)
C6′—C5′—C4′	118.70 (14)	C12′—C11′—H11A	109.1
C6′—C5′—H5′	120.6	C10′—C11′—H11A	109.1
C4′—C5′—H5′	120.6	C12′—C11′—H11B	109.1
C6—C5—C4	118.94 (17)	C10′—C11′—H11B	109.1
C6—C5—H5	120.5	H11A—C11′—H11B	107.9
C4—C5—H5	120.5	C12—C11—C10	112.34 (14)
C5′—C6′—C7′	121.46 (16)	C12—C11—H11C	109.1
C5′—C6′—H6′	119.3	C10—C11—H11C	109.1
C7′—C6′—H6′	119.3	C12—C11—H11D	109.1
C5—C6—C7	121.09 (19)	C10—C11—H11D	109.1
C5—C6—H6	119.5	H11C—C11—H11D	107.9
C7—C6—H6	119.5	N13—C12—C11	179.8 (2)
C8′—C7′—C6′	121.15 (16)	N13′—C12′—C11′	179.6 (2)

C9—N1—C2—C3	0.0 (2)	C2—N1—C9—C4	0.35 (18)
C9′—N1′—C2′—C3′	0.34 (17)	C5—C4—C9—C8	−0.7 (2)
N1—C2—C3—C10	178.76 (15)	C3—C4—C9—C8	179.28 (15)
N1—C2—C3—C4	−0.41 (19)	C5—C4—C9—N1	179.39 (14)
N1′—C2′—C3′—C10′	179.69 (14)	C3—C4—C9—N1	−0.59 (17)
N1′—C2′—C3′—C4′	−0.69 (17)	C2′—N1′—C9′—C8′	179.31 (16)
C2—C3—C4—C5	−179.36 (17)	C2′—N1′—C9′—C4′	0.18 (17)
C10—C3—C4—C5	1.5 (3)	C7′—C8′—C9′—N1′	−177.93 (15)
C2—C3—C4—C9	0.61 (17)	C7′—C8′—C9′—C4′	1.1 (2)
C10—C3—C4—C9	−178.56 (15)	C5′—C4′—C9′—N1′	177.78 (13)
C2′—C3′—C4′—C5′	−177.20 (16)	C3′—C4′—C9′—N1′	−0.59 (16)
C10′—C3′—C4′—C5′	2.4 (3)	C5′—C4′—C9′—C8′	−1.4 (2)
C2′—C3′—C4′—C9′	0.78 (16)	C3′—C4′—C9′—C8′	−179.80 (14)
C10′—C3′—C4′—C9′	−179.60 (14)	C2—C3—C10—O1	−179.17 (16)
C9′—C4′—C5′—C6′	0.4 (2)	C4—C3—C10—O1	−0.2 (3)
C3′—C4′—C5′—C6′	178.23 (16)	C2—C3—C10—C11	0.1 (2)
C9—C4—C5—C6	0.2 (2)	C4—C3—C10—C11	179.09 (15)
C3—C4—C5—C6	−179.88 (17)	C2′—C3′—C10′—O1′	−179.31 (15)
C4′—C5′—C6′—C7′	0.8 (3)	C4′—C3′—C10′—O1′	1.1 (2)

C4—C5—C6—C7	0.6 (3)	C2′—C3′—C10′—C11′	−0.3 (2)
C5′—C6′—C7′—C8′	−1.2 (3)	C4′—C3′—C10′—C11′	−179.83 (13)
C5—C6—C7—C8	−0.9 (3)	O1′—C10′—C11′—C12′	−14.8 (2)
C6′—C7′—C8′—C9′	0.2 (3)	C3′—C10′—C11′—C12′	166.12 (13)
C6—C7—C8—C9	0.3 (3)	O1—C10—C11—C12	−2.2 (2)
C7—C8—C9—N1	−179.67 (17)	C3—C10—C11—C12	178.56 (15)
C7—C8—C9—C4	0.5 (3)	C10—C11—C12—N13	51 (88)
C2—N1—C9—C8	−179.50 (18)	C10′—C11′—C12′—N13′	−58 (25)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	1.98	2.8146 (18)	163
C2—H2···N13^{i}	0.93	2.59	3.236 (2)	127
N1′—H1′···O1′^{ii}	0.86	2.00	2.8166 (15)	158

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