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4-Cyano-3,5-bis(phenyl)pyrazole

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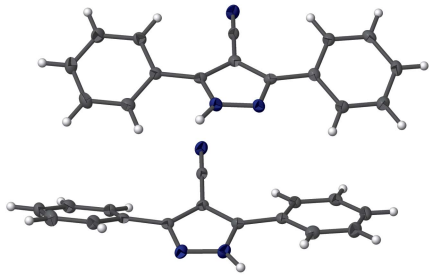
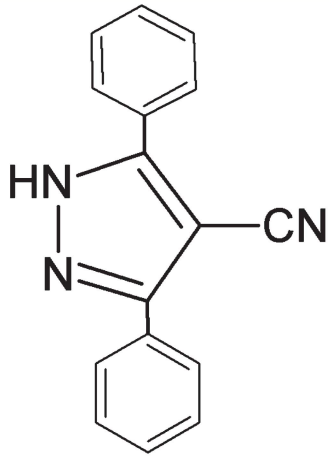
There are two independent molecules in the asymmetric unit of the title compound, $C_{16}H_{11}N_3$. The molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers with an R_2^2 (6) ring motif.

3D view



Chemical scheme



Structure description

The title compound, representing a symmetrically phenyl substituted 4-cyano pyrazole, was prepared as a precursor for the preparation of scorpionate ligands (Trofimenko, 1999). There are two molecules in the asymmetric unit. The C—C≡N fragments deviate only slightly from linearity with a bonding angle of 179.4 (2)° (N1—C1—C2) and 178.9 (2)° (N1′—C1′—C2′) (Fig. 1). The dihedral angles between one pyrazole ring (N2/N3/C2–C4) and the mean planes of the two phenyl rings are 21.26° (C5–C10) and 24.31° (C11–C16) in one molecule of the asymmetric unit. In the other molecule, the dihedral angles between the pyrazole ring (N2′/N3′/C2′–C4′) and the mean planes of the two phenyl rings are 19.72° (C5′–C10′) and 34.39° (C11′–C16′).

In the crystal, molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers with an R_2^2 (6) ring motif (Fig. 2 and Table 1). There are no other significant intermolecular interactions present.

Synthesis and crystallization

Toluene was dried over sodium and benzophenone. All other solvents and reagents were used as received from Alfa Aesar or Fisher Scientific without further purification. The synthesis of 4-cyano-3,5-bisphenyl pyrazole has been reported (Som, 2013). The procedure was modified in this work to recrystallize the final product. 0.69 g (17.24 mmol, 60% dispersion in mineral oil) of sodium hydride was added to 100 ml dry toluene. To this solution was added 2.50 g of benzoylacetonitrile (17.24 mmol), resulting in the immediate appearance of bubbles. The mixture was stirred for 18 h before benzoyl chloride (2.43 g, 17.24 mmol) was added. The reaction mixture was stirred overnight followed by three

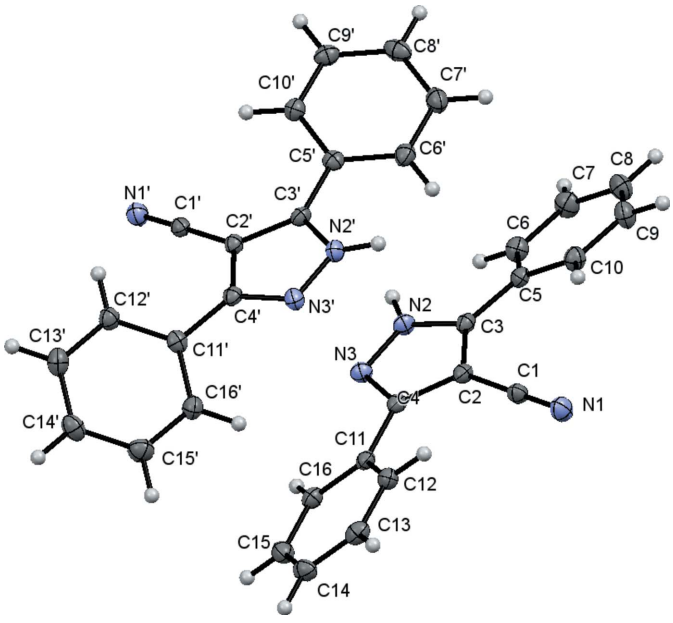


Figure 1
A view of the asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii.

extractions using 100 ml of 0.2 *M* NaOH solution each time. The aqueous layers were combined and acidified with HCl/H_2O (50/50) solution to pH ~1. A white precipitate appeared immediately and was extracted with three 100 ml portions of ethyl acetate. Removal of the solvent under reduced pressure yielded 2.55 g (10.24 mmol, yield 59.40%) of crude product, which was recrystallized from ethanol to give 2-cyano-1,3-diphenyl-1,3-propanedione (1.38 g, 5.54 mmol, 32.15%). This diketone compound (1.38 g, 5.54 mmol) was then reacted with hydrazine monohydrate (0.28 g, 5.54 mmol) in 100 ml of methanol and stirred overnight. The solvent was removed under reduced pressure to yield the crude product of 4-cyano-3,5-bisphenyl pyrazole as a pale-yellow solid, which was recrystallized from ethanol (1.01 g, 4.65 mmol, 27.00%). Infrared spectroscopy showed characteristic peaks at 3177 cm^{-1} and 2227 cm^{-1} for N—H and C≡N stretches respectively. The ^{1}H NMR (chloroform-*d*) showed chemical shifts at 8.06 (*d*, 4H), 7.64 (*t*, 4H), and 7.54 p.p.m. (*t*, 2H).

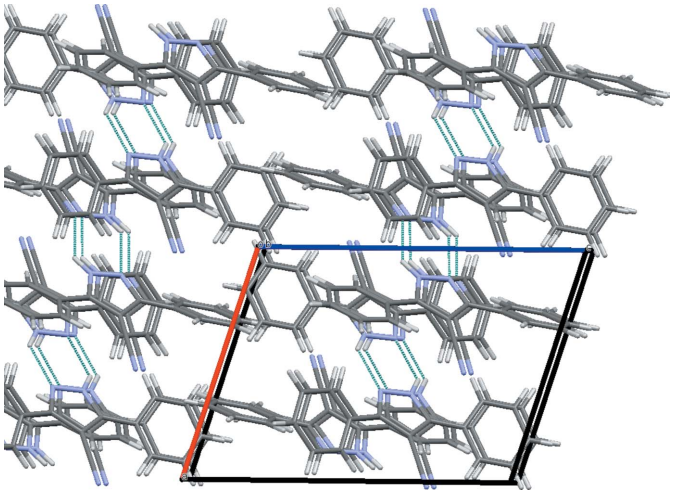


Figure 2
A view along the *b* axis of the crystal packing of the title compound. The N—H···N hydrogen bonds (Table 1) are shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N3^{i}	0.88	2.13	2.812 (2)	133
N2′—H2′···N3′^{ii}	0.88	2.13	2.793 (2)	131

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{11}N_3$
M_r	245.28
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	9.6036 (7), 10.4998 (6), 13.4359 (7)
α, β, γ (°)	104.899 (2), 106.704 (2), 90.647 (2)
V (Å^3)	1248.70 (13)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.08
Crystal size (mm)	0.25 × 0.24 × 0.16
Data collection	
Diffractometer	Bruker X8 *APEX* II
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.235, 0.260
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25032, 5069, 3178
R_{int}	0.050
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.122, 1.02
No. of reflections	5069
No. of parameters	343
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.29

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

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

Acknowledgements

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full crystallographic data

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Crystal data

$C_{16}H_{11}N_3$
$M_r = 245.28$
Triclinic, $P\overline{1}$
$a = 9.6036$ (7) Å
$b = 10.4998$ (6) Å
$c = 13.4359$ (7) Å
$\alpha = 104.899$ (2)°
$\beta = 106.704$ (2)°
$\gamma = 90.647$ (2)°
$V = 1248.70$ (13) Å^3
$Z = 4$
$F(000) = 512$
$D_x = 1.305$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2987 reflections
$\theta = 2.9$–$26.3°$
$\mu = 0.08$ mm^{-1}
$T = 100$ K
Block, colourless
0.25 × 0.24 × 0.16 mm

Data collection

Bruker X8 APEX II diffractometer
Radiation source: sealed tube, fine-focus
Graphite monochromator
Detector resolution: 7.9 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min} = 0.235$, $T_{max} = 0.260$
25032 measured reflections
5069 independent reflections
3178 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.3°$
$h = -12 \rightarrow 11$
$k = -11 \rightarrow 13$
$l = -16 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.122$
$S = 1.02$
5069 reflections
343 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.1764P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	−0.02188 (18)	0.73573 (16)	0.25572 (13)	0.0251 (4)
N2	0.37446 (17)	0.51162 (15)	0.39966 (12)	0.0186 (4)
H2	0.433514	0.448492	0.393834	0.022*
N3	0.38722 (16)	0.60550 (15)	0.49310 (12)	0.0179 (4)
C1	0.0762 (2)	0.69081 (18)	0.30236 (15)	0.0176 (4)
C2	0.1967 (2)	0.63420 (17)	0.36031 (14)	0.0162 (4)
C3	0.2628 (2)	0.52451 (17)	0.31689 (14)	0.0155 (4)
C4	0.27925 (19)	0.68260 (17)	0.47057 (14)	0.0154 (4)
C5	0.2349 (2)	0.43615 (18)	0.20816 (14)	0.0164 (4)
C6	0.3463 (2)	0.36427 (19)	0.17986 (15)	0.0213 (5)
H6	0.440196	0.374746	0.231165	0.026*
C7	0.3211 (2)	0.2782 (2)	0.07803 (16)	0.0254 (5)
H7	0.397375	0.229588	0.060013	0.031*
C8	0.1852 (2)	0.2628 (2)	0.00262 (16)	0.0265 (5)
H8	0.167909	0.203569	−0.067200	0.032*
C9	0.0740 (2)	0.3338 (2)	0.02888 (15)	0.0252 (5)
H9	−0.019124	0.324002	−0.023297	0.030*
C10	0.0983 (2)	0.41922 (19)	0.13107 (14)	0.0211 (5)
H10	0.021178	0.466678	0.148755	0.025*
C11	0.2659 (2)	0.79827 (17)	0.55498 (14)	0.0161 (4)
C12	0.1333 (2)	0.85396 (18)	0.55028 (15)	0.0181 (4)
H12	0.048672	0.816321	0.491553	0.022*
C13	0.1247 (2)	0.96388 (18)	0.63099 (15)	0.0204 (4)
H13	0.034133	1.000761	0.627423	0.024*
C14	0.2476 (2)	1.02033 (19)	0.71690 (15)	0.0221 (5)
H14	0.241423	1.095891	0.771824	0.026*
C15	0.3795 (2)	0.96562 (19)	0.72200 (15)	0.0217 (5)
H15	0.463800	1.004018	0.780711	0.026*
C16	0.3891 (2)	0.85577 (18)	0.64240 (14)	0.0184 (4)
H16	0.479864	0.818935	0.646943	0.022*
N1′	0.46981 (18)	0.72545 (15)	0.25682 (12)	0.0225 (4)
N2′	0.87772 (17)	0.59563 (15)	0.49062 (12)	0.0192 (4)
H2′	0.940673	0.601874	0.554283	0.023*
N3′	0.87116 (17)	0.50046 (15)	0.39906 (12)	0.0192 (4)
C1′	0.5726 (2)	0.68557 (17)	0.30272 (14)	0.0163 (4)
C2′	0.69826 (19)	0.63418 (17)	0.35991 (14)	0.0155 (4)
C3′	0.7753 (2)	0.67868 (17)	0.47078 (14)	0.0156 (4)
C4′	0.7634 (2)	0.52153 (17)	0.31792 (14)	0.0154 (4)
C5′	0.7632 (2)	0.79276 (18)	0.55686 (14)	0.0168 (4)
C6′	0.8279 (2)	0.79538 (19)	0.66520 (15)	0.0206 (5)
H6′	0.874686	0.721159	0.682310	0.025*
C7′	0.8244 (2)	0.90496 (19)	0.74751 (16)	0.0245 (5)
H7′	0.868809	0.905714	0.820647	0.029*
C8′	0.7563 (2)	1.01351 (19)	0.72334 (16)	0.0238 (5)
H8′	0.754213	1.088901	0.779799	0.029*

C9′	0.6910 (2)	1.01187 (19)	0.61653 (15)	0.0206 (4)
H9′	0.643333	1.085992	0.600059	0.025*
C10′	0.6948 (2)	0.90301 (18)	0.53375 (15)	0.0181 (4)
H10′	0.650589	0.903232	0.460816	0.022*
C11′	0.73338 (19)	0.43430 (18)	0.20814 (14)	0.0164 (4)
C12′	0.6884 (2)	0.48498 (19)	0.11845 (14)	0.0189 (4)
H12′	0.674383	0.576273	0.128153	0.023*
C13′	0.6642 (2)	0.4018 (2)	0.01540 (15)	0.0230 (5)
H13′	0.634018	0.436559	−0.045343	0.028*
C14′	0.6837 (2)	0.2686 (2)	0.00036 (15)	0.0242 (5)
H14′	0.665821	0.211888	−0.070494	0.029*
C15′	0.7295 (2)	0.2180 (2)	0.08919 (16)	0.0254 (5)
H15′	0.743772	0.126708	0.078976	0.030*
C16′	0.7545 (2)	0.29997 (18)	0.19248 (15)	0.0207 (4)
H16′	0.786021	0.264849	0.252923	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0250 (10)	0.0233 (9)	0.0222 (9)	0.0065 (8)	0.0012 (8)	0.0043 (8)
N2	0.0189 (9)	0.0168 (9)	0.0200 (9)	0.0067 (7)	0.0053 (7)	0.0051 (7)
N3	0.0183 (9)	0.0166 (9)	0.0187 (9)	0.0044 (7)	0.0059 (7)	0.0042 (7)
C1	0.0193 (11)	0.0155 (10)	0.0166 (10)	0.0027 (9)	0.0050 (9)	0.0020 (8)
C2	0.0159 (10)	0.0156 (10)	0.0180 (10)	0.0015 (8)	0.0048 (8)	0.0066 (8)
C3	0.0132 (10)	0.0169 (10)	0.0170 (10)	0.0016 (8)	0.0028 (8)	0.0075 (8)
C4	0.0135 (10)	0.0153 (10)	0.0182 (10)	0.0012 (8)	0.0037 (8)	0.0074 (8)
C5	0.0179 (10)	0.0169 (10)	0.0159 (10)	0.0016 (8)	0.0057 (8)	0.0066 (8)
C6	0.0194 (11)	0.0243 (11)	0.0217 (11)	0.0035 (9)	0.0072 (9)	0.0079 (9)
C7	0.0291 (12)	0.0269 (12)	0.0234 (11)	0.0085 (10)	0.0133 (10)	0.0058 (9)
C8	0.0326 (13)	0.0278 (12)	0.0177 (11)	0.0028 (10)	0.0084 (10)	0.0028 (9)
C9	0.0240 (12)	0.0313 (12)	0.0171 (11)	0.0037 (9)	0.0023 (9)	0.0054 (9)
C10	0.0203 (11)	0.0234 (11)	0.0202 (11)	0.0047 (9)	0.0061 (9)	0.0065 (9)
C11	0.0193 (11)	0.0150 (10)	0.0161 (10)	0.0030 (8)	0.0062 (8)	0.0069 (8)
C12	0.0197 (11)	0.0181 (10)	0.0168 (10)	0.0016 (8)	0.0053 (8)	0.0055 (8)
C13	0.0205 (11)	0.0210 (11)	0.0244 (11)	0.0062 (9)	0.0110 (9)	0.0094 (9)
C14	0.0291 (12)	0.0179 (10)	0.0204 (11)	0.0025 (9)	0.0118 (9)	0.0026 (9)
C15	0.0223 (11)	0.0215 (11)	0.0192 (11)	−0.0011 (9)	0.0043 (9)	0.0041 (9)
C16	0.0182 (11)	0.0186 (10)	0.0198 (10)	0.0036 (8)	0.0054 (9)	0.0077 (9)
N1′	0.0234 (10)	0.0217 (9)	0.0192 (9)	0.0034 (8)	0.0023 (8)	0.0043 (7)
N2′	0.0192 (9)	0.0195 (9)	0.0161 (9)	0.0021 (7)	0.0005 (7)	0.0052 (7)
N3′	0.0202 (9)	0.0202 (9)	0.0149 (9)	0.0000 (7)	0.0022 (7)	0.0046 (7)
C1′	0.0190 (11)	0.0151 (10)	0.0145 (10)	−0.0002 (8)	0.0052 (8)	0.0035 (8)
C2′	0.0136 (10)	0.0167 (10)	0.0156 (10)	0.0007 (8)	0.0028 (8)	0.0057 (8)
C3′	0.0149 (10)	0.0150 (10)	0.0183 (10)	0.0028 (8)	0.0046 (8)	0.0072 (8)
C4′	0.0146 (10)	0.0161 (10)	0.0166 (10)	0.0002 (8)	0.0045 (8)	0.0065 (8)
C5′	0.0152 (10)	0.0178 (10)	0.0180 (10)	−0.0004 (8)	0.0061 (8)	0.0047 (8)
C6′	0.0212 (11)	0.0222 (11)	0.0201 (11)	0.0010 (9)	0.0056 (9)	0.0093 (9)
C7′	0.0274 (12)	0.0279 (12)	0.0171 (10)	−0.0013 (9)	0.0059 (9)	0.0054 (9)

C8′	0.0255 (12)	0.0213 (11)	0.0239 (11)	−0.0027 (9)	0.0125 (9)	−0.0006 (9)
C9′	0.0194 (11)	0.0180 (10)	0.0264 (11)	0.0030 (8)	0.0091 (9)	0.0072 (9)
C10′	0.0173 (10)	0.0196 (10)	0.0183 (10)	0.0023 (8)	0.0061 (8)	0.0061 (9)
C11′	0.0116 (10)	0.0200 (10)	0.0170 (10)	0.0021 (8)	0.0041 (8)	0.0040 (8)
C12′	0.0178 (11)	0.0202 (10)	0.0180 (10)	0.0038 (8)	0.0036 (8)	0.0056 (9)
C13′	0.0209 (11)	0.0308 (12)	0.0182 (10)	0.0054 (9)	0.0057 (9)	0.0085 (9)
C14′	0.0236 (12)	0.0272 (12)	0.0191 (11)	0.0039 (9)	0.0071 (9)	0.0006 (9)
C15′	0.0292 (12)	0.0205 (11)	0.0266 (12)	0.0056 (9)	0.0104 (10)	0.0046 (9)
C16′	0.0226 (11)	0.0228 (11)	0.0175 (10)	0.0024 (9)	0.0056 (9)	0.0072 (9)

Geometric parameters (Å, º)

N1—C1	1.151 (2)	N1′—C1′	1.150 (2)
N2—H2	0.8800	N2′—H2′	0.8800
N2—N3	1.355 (2)	N2′—N3′	1.356 (2)
N2—C3	1.342 (2)	N2′—C3′	1.337 (2)
N3—C4	1.337 (2)	N3′—C4′	1.338 (2)
C1—C2	1.426 (3)	C1′—C2′	1.426 (3)
C2—C3	1.398 (2)	C2′—C3′	1.409 (2)
C2—C4	1.418 (2)	C2′—C4′	1.409 (2)
C3—C5	1.463 (3)	C3′—C5′	1.468 (3)
C4—C11	1.468 (3)	C4′—C11′	1.467 (3)
C5—C6	1.401 (3)	C5′—C6′	1.402 (2)
C5—C10	1.394 (3)	C5′—C10′	1.398 (2)
C6—H6	0.9500	C6′—H6′	0.9500
C6—C7	1.384 (3)	C6′—C7′	1.384 (3)
C7—H7	0.9500	C7′—H7′	0.9500
C7—C8	1.381 (3)	C7′—C8′	1.385 (3)
C8—H8	0.9500	C8′—H8′	0.9500
C8—C9	1.385 (3)	C8′—C9′	1.387 (3)
C9—H9	0.9500	C9′—H9′	0.9500
C9—C10	1.386 (3)	C9′—C10′	1.384 (3)
C10—H10	0.9500	C10′—H10′	0.9500
C11—C12	1.400 (3)	C11′—C12′	1.399 (2)
C11—C16	1.401 (3)	C11′—C16′	1.397 (3)
C12—H12	0.9500	C12′—H12′	0.9500
C12—C13	1.387 (3)	C12′—C13′	1.386 (3)
C13—H13	0.9500	C13′—H13′	0.9500
C13—C14	1.387 (3)	C13′—C14′	1.384 (3)
C14—H14	0.9500	C14′—H14′	0.9500
C14—C15	1.388 (3)	C14′—C15′	1.389 (3)
C15—H15	0.9500	C15′—H15′	0.9500
C15—C16	1.381 (3)	C15′—C16′	1.383 (3)
C16—H16	0.9500	C16′—H16′	0.9500
N3—N2—H2	123.4	N3′—N2′—H2′	124.7
C3—N2—H2	123.4	C3′—N2′—H2′	124.7
C3—N2—N3	113.27 (15)	C3′—N2′—N3′	110.59 (15)

C4—N3—N2	106.08 (14)	C4′—N3′—N2′	108.59 (15)
N1—C1—C2	179.40 (19)	N1′—C1′—C2′	178.85 (18)
C3—C2—C1	126.21 (16)	C3′—C2′—C1′	127.30 (17)
C3—C2—C4	106.48 (15)	C4′—C2′—C1′	126.42 (16)
C4—C2—C1	127.18 (17)	C4′—C2′—C3′	106.12 (15)
N2—C3—C2	105.10 (16)	N2′—C3′—C2′	106.76 (16)
N2—C3—C5	121.48 (17)	N2′—C3′—C5′	120.83 (16)
C2—C3—C5	133.38 (17)	C2′—C3′—C5′	132.37 (16)
N3—C4—C2	109.06 (16)	N3′—C4′—C2′	107.95 (16)
N3—C4—C11	119.72 (16)	N3′—C4′—C11′	120.35 (17)
C2—C4—C11	131.19 (16)	C2′—C4′—C11′	131.69 (16)
C6—C5—C3	119.99 (17)	C6′—C5′—C3′	119.77 (16)
C10—C5—C3	121.67 (17)	C10′—C5′—C3′	121.56 (16)
C10—C5—C6	118.34 (17)	C10′—C5′—C6′	118.58 (17)
C5—C6—H6	119.6	C5′—C6′—H6′	119.7
C7—C6—C5	120.81 (18)	C7′—C6′—C5′	120.69 (17)
C7—C6—H6	119.6	C7′—C6′—H6′	119.7
C6—C7—H7	120.0	C6′—C7′—H7′	120.0
C8—C7—C6	120.07 (19)	C6′—C7′—C8′	120.06 (18)
C8—C7—H7	120.0	C8′—C7′—H7′	120.0
C7—C8—H8	120.0	C7′—C8′—H8′	120.1
C7—C8—C9	119.94 (19)	C7′—C8′—C9′	119.83 (18)
C9—C8—H8	120.0	C9′—C8′—H8′	120.1
C8—C9—H9	119.9	C8′—C9′—H9′	119.8
C8—C9—C10	120.19 (19)	C10′—C9′—C8′	120.47 (18)
C10—C9—H9	119.9	C10′—C9′—H9′	119.8
C5—C10—H10	119.7	C5′—C10′—H10′	119.8
C9—C10—C5	120.66 (19)	C9′—C10′—C5′	120.36 (17)
C9—C10—H10	119.7	C9′—C10′—H10′	119.8
C12—C11—C4	121.76 (17)	C12′—C11′—C4′	120.66 (16)
C12—C11—C16	118.72 (17)	C16′—C11′—C4′	120.00 (15)
C16—C11—C4	119.52 (17)	C16′—C11′—C12′	119.30 (17)
C11—C12—H12	119.9	C11′—C12′—H12′	120.0
C13—C12—C11	120.28 (18)	C13′—C12′—C11′	119.92 (17)
C13—C12—H12	119.9	C13′—C12′—H12′	120.0
C12—C13—H13	119.8	C12′—C13′—H13′	119.8
C12—C13—C14	120.48 (18)	C14′—C13′—C12′	120.49 (17)
C14—C13—H13	119.8	C14′—C13′—H13′	119.8
C13—C14—H14	120.2	C13′—C14′—H14′	120.1
C13—C14—C15	119.52 (19)	C13′—C14′—C15′	119.80 (18)
C15—C14—H14	120.2	C15′—C14′—H14′	120.1
C14—C15—H15	119.7	C14′—C15′—H15′	119.9
C16—C15—C14	120.51 (19)	C16′—C15′—C14′	120.29 (18)
C16—C15—H15	119.7	C16′—C15′—H15′	119.9
C11—C16—H16	119.8	C11′—C16′—H16′	119.9
C15—C16—C11	120.49 (18)	C15′—C16′—C11′	120.18 (17)
C15—C16—H16	119.8	C15′—C16′—H16′	119.9

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N3^{i}	0.88	2.13	2.812 (2)	133
N2′—H2′···N3′^{ii}	0.88	2.13	2.793 (2)	131

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