

4-(5-Phenyl-1,2,4-triazolo[3,4-a]-isoquinolin-3-yl)benzonitrile

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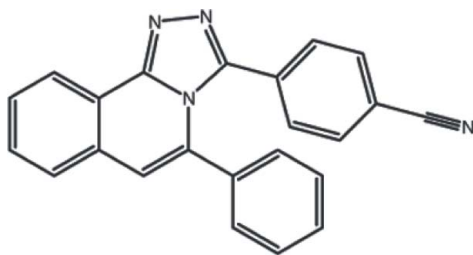
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Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.046; wR factor = 0.100; data-to-parameter ratio = 13.0.

In the title molecule, $\text{C}_{23}\text{H}_{14}\text{N}_4$, the triazoloisoquinoline ring system is nearly planar, with an r.m.s. deviation of 0.038 (2) Å and a maximum deviation of -0.030 (2) Å from the mean plane of the triazole ring C atom which is bonded to the benzene ring. The benzene and phenyl rings are twisted by 57.65 (8) and 53.60 (9)°, respectively, with respect to the mean plane of the triazoloisoquinoline ring system. In the crystal structure, molecules are linked by weak aromatic $\pi-\pi$ interactions [centroid-centroid distance = 3.8074 (12) Å]. In addition, the crystal structure exhibits a nonclassical intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bond.

Related literature

For a related crystal structure, see: Khan *et al.* (2010).

Experimental

Crystal data

$\text{C}_{23}\text{H}_{14}\text{N}_4$	$V = 3421.5$ (2) Å ³
$M_r = 346.38$	$Z = 8$
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
$a = 7.1614$ (3) Å	$\mu = 0.08$ mm ⁻¹
$b = 18.0957$ (7) Å	$T = 290$ K
$c = 26.4021$ (9) Å	$0.25 \times 0.21 \times 0.17$ mm

Data collection

Oxford Xcalibur Eos (Nova) CCD detector diffractometer	14977 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO RED</i> ; Oxford Diffraction, 2009)	3164 independent reflections
$T_{\min} = 0.959$, $T_{\max} = 0.986$	1490 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.070$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$	244 parameters
$wR(F^2) = 0.100$	H-atom parameters constrained
$S = 0.81$	$\Delta\rho_{\text{max}} = 0.15$ e Å ⁻³
3164 reflections	$\Delta\rho_{\text{min}} = -0.20$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C11}-\text{H11}\cdots\text{N3}^i$	0.93	2.50	3.418 (3)	170

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

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2009); 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: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2199).

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supplementary materials

Acta Cryst. (2010). E66, o1081 [doi:10.1107/S1600536810013012]

4-(5-Phenyl-1,2,4-triazolo[3,4-*a*]isoquinolin-3-yl)benzotrile

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Comment

As part of our search for new isoquinoline analogues (Khan *et al.*, 2010), we focused on synthesis of titled compounds and the crystal structure is reported.

In the title molecule, Fig. 1, the triazoloisoquinoline ring system (N1-N3/C1-C9/C16) is nearly planar, with an r.m.s. deviation of 0.038 (2) Å and a maximum deviation of -0.030 (2) Å from the mean plane for the triazole ring C16 atom which is bonded to the benzene ring (C17-C22). The benzene (C17-C22) and phenyl (C10-C15) rings are twisted by 57.65 (8)° and 53.60 (9)°, respectively, with respect to the mean plane of the triazoloisoquinoline ring system. The benzene (C17-C22) and phenyl (C10-C15) rings make a dihedral angle of 29.10 (11)° with each other.

Molecular conformation is stabilized by a weak π - π interaction [Cg4...Cg5 = 3.8229 (14) Å, where are Cg4 and Cg5 are centroids of the C10-C15 and C17-C22 rings, respectively]. In the crystal structure, the molecules are linked by weak aromatic π - π interactions [Cg1...Cg1ⁱⁱ = 3.8074 (12) Å, symmetry code: (ii) $x-1/2, 1/2-y, -z$. Cg1 is the centroid of the N1-N3/C1/C16 ring]. In addition, the crystal structure exhibits an intermolecular non-classical C-H...N hydrogen bond (Table 1, Fig. 2).

Experimental

2-(3-Phenylisoquinolin-1-yl)hydrazine (1 mmol) was condensed with 4-formylbenzotrile (1.1 mmol) under refluxing conditions isopropanol (10 ml) solvent to give the corresponding hydrazone in high yield. After removal of solvent the compound was then oxidatively cyclized in nitrobenzene (10 ml) at 473 K. The product was recrystallized from dichloromethane to give block-shaped crystals.

Refinement

All H atoms were placed in calculated positions with C-H = 0.93 Å and were included in the refinement in the riding model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Pure diffraction experiment (ratio observed/unique reflections 47%) we explain by weak diffraction of the crystal.

Figures

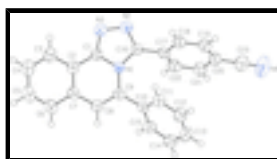


Fig. 1. The view of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

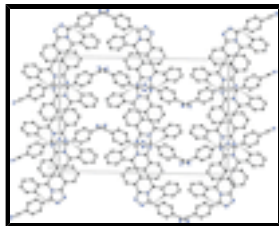


Fig. 2. The packing diagram and the hydrogen bonding in the title crystal structure viewed down the [1 0 0] direction. H atoms not involved in the motif shown have been omitted for clarity.

(I)

Crystal data

$C_{23}H_{14}N_4$

$M_r = 346.38$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 7.1614 (3) \text{ \AA}$

$b = 18.0957 (7) \text{ \AA}$

$c = 26.4021 (9) \text{ \AA}$

$V = 3421.5 (2) \text{ \AA}^3$

$Z = 8$

$F(000) = 1440$

$D_x = 1.345 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1235 reflections

$\theta = 1.6\text{--}20.4^\circ$

$\mu = 0.08 \text{ mm}^{-1}$

$T = 290 \text{ K}$

Block, colourless

$0.25 \times 0.21 \times 0.17 \text{ mm}$

Data collection

Oxford Xcalibur Eos (Nova) CCD detector diffractometer

Radiation source: Enhance (Mo) X-ray Source graphite

ω scans

Absorption correction: multi-scan (*CrysAlis Pro RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.959$, $T_{\max} = 0.986$

14977 measured reflections

3164 independent reflections

1490 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.070$

$\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 3.1^\circ$

$h = -8 \rightarrow 7$

$k = -21 \rightarrow 21$

$l = -31 \rightarrow 31$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.100$

$S = 0.81$

3164 reflections

244 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

$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.15 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.20 \text{ e \AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.6627 (2)	0.33099 (9)	0.03366 (6)	0.0370 (4)
N2	0.5820 (3)	0.22467 (10)	-0.00072 (7)	0.0510 (5)
N3	0.6063 (2)	0.27481 (11)	-0.03950 (7)	0.0495 (5)
N4	0.5390 (3)	0.08980 (15)	0.27259 (9)	0.0927 (9)
C1	0.6539 (3)	0.33812 (13)	-0.01851 (8)	0.0395 (5)
C2	0.6915 (3)	0.40722 (12)	-0.04237 (8)	0.0407 (6)
C3	0.6888 (3)	0.41638 (14)	-0.09495 (8)	0.0490 (6)
H3	0.6586	0.3766	-0.1157	0.059*
C4	0.7302 (3)	0.48368 (15)	-0.11611 (9)	0.0570 (7)
H4	0.7297	0.4894	-0.1511	0.068*
C5	0.7728 (3)	0.54308 (14)	-0.08507 (9)	0.0581 (7)
H5	0.8002	0.5887	-0.0996	0.070*
C6	0.7754 (3)	0.53585 (13)	-0.03328 (9)	0.0526 (6)
H6	0.8030	0.5764	-0.0130	0.063*
C7	0.7364 (3)	0.46741 (12)	-0.01110 (8)	0.0416 (6)
C8	0.7527 (3)	0.45523 (12)	0.04249 (8)	0.0454 (6)
H8	0.7853	0.4952	0.0628	0.054*
C9	0.7238 (3)	0.38972 (12)	0.06498 (8)	0.0387 (6)
C10	0.7671 (3)	0.37673 (11)	0.11909 (8)	0.0374 (5)
C11	0.8907 (3)	0.32192 (12)	0.13406 (8)	0.0456 (6)
H11	0.9426	0.2903	0.1101	0.055*
C12	0.9365 (3)	0.31454 (14)	0.18466 (9)	0.0562 (7)
H12	1.0180	0.2774	0.1948	0.067*
C13	0.8625 (4)	0.36161 (15)	0.22007 (9)	0.0645 (8)
H13	0.8935	0.3561	0.2541	0.077*
C14	0.7438 (4)	0.41647 (15)	0.20553 (9)	0.0595 (7)
H14	0.6960	0.4490	0.2295	0.071*
C15	0.6944 (3)	0.42380 (13)	0.15537 (9)	0.0478 (6)
H15	0.6114	0.4608	0.1458	0.057*
C16	0.6137 (3)	0.25837 (12)	0.04252 (8)	0.0406 (6)
C17	0.5906 (3)	0.22246 (12)	0.09194 (8)	0.0403 (5)
C18	0.6918 (3)	0.15870 (13)	0.10218 (8)	0.0480 (6)
H18	0.7701	0.1391	0.0775	0.058*

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C19	0.6771 (3)	0.12414 (12)	0.14857 (9)	0.0523 (6)
H19	0.7474	0.0821	0.1554	0.063*
C20	0.5575 (3)	0.15217 (13)	0.18497 (8)	0.0480 (6)
C21	0.4514 (3)	0.21414 (13)	0.17476 (8)	0.0524 (6)
H21	0.3693	0.2324	0.1990	0.063*
C22	0.4678 (3)	0.24882 (13)	0.12834 (8)	0.0503 (6)
H22	0.3957	0.2903	0.1214	0.060*
C23	0.5459 (3)	0.11720 (15)	0.23405 (10)	0.0629 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0393 (10)	0.0337 (11)	0.0381 (11)	-0.0026 (8)	-0.0031 (8)	-0.0012 (9)
N2	0.0631 (13)	0.0439 (12)	0.0459 (12)	-0.0068 (10)	-0.0062 (10)	-0.0041 (11)
N3	0.0614 (13)	0.0457 (13)	0.0414 (11)	-0.0057 (10)	-0.0054 (9)	0.0003 (10)
N4	0.0964 (19)	0.124 (2)	0.0576 (16)	0.0151 (16)	0.0099 (14)	0.0261 (16)
C1	0.0394 (14)	0.0404 (15)	0.0387 (13)	-0.0003 (11)	-0.0054 (10)	-0.0027 (12)
C2	0.0357 (13)	0.0443 (15)	0.0421 (14)	0.0023 (11)	-0.0010 (10)	0.0016 (12)
C3	0.0463 (15)	0.0544 (17)	0.0463 (15)	0.0062 (13)	0.0002 (11)	0.0032 (13)
C4	0.0515 (17)	0.0687 (19)	0.0507 (15)	0.0085 (14)	0.0028 (12)	0.0160 (15)
C5	0.0464 (16)	0.0584 (19)	0.0695 (19)	-0.0011 (13)	-0.0002 (13)	0.0241 (15)
C6	0.0500 (15)	0.0465 (16)	0.0613 (17)	-0.0003 (12)	-0.0016 (13)	0.0076 (13)
C7	0.0344 (14)	0.0413 (15)	0.0490 (14)	0.0004 (11)	-0.0046 (11)	0.0072 (12)
C8	0.0461 (14)	0.0387 (15)	0.0513 (15)	-0.0011 (11)	-0.0052 (12)	-0.0054 (12)
C9	0.0347 (14)	0.0368 (15)	0.0445 (13)	-0.0002 (10)	-0.0019 (11)	-0.0060 (11)
C10	0.0399 (14)	0.0336 (13)	0.0386 (13)	-0.0029 (11)	-0.0012 (10)	-0.0018 (11)
C11	0.0441 (14)	0.0436 (15)	0.0492 (15)	-0.0011 (12)	-0.0005 (11)	-0.0047 (12)
C12	0.0519 (16)	0.0604 (18)	0.0563 (17)	0.0036 (13)	-0.0129 (13)	0.0072 (15)
C13	0.075 (2)	0.077 (2)	0.0416 (15)	-0.0091 (16)	-0.0111 (14)	0.0000 (15)
C14	0.0721 (18)	0.0580 (18)	0.0483 (16)	-0.0068 (15)	0.0073 (14)	-0.0115 (14)
C15	0.0507 (15)	0.0429 (15)	0.0497 (15)	0.0013 (12)	0.0008 (12)	-0.0051 (13)
C16	0.0436 (14)	0.0361 (14)	0.0423 (13)	-0.0039 (11)	-0.0025 (11)	-0.0031 (12)
C17	0.0400 (13)	0.0351 (14)	0.0458 (14)	-0.0048 (11)	-0.0039 (11)	-0.0015 (11)
C18	0.0586 (15)	0.0392 (15)	0.0463 (15)	0.0034 (13)	0.0039 (12)	-0.0031 (12)
C19	0.0637 (17)	0.0400 (15)	0.0532 (16)	0.0085 (12)	0.0004 (13)	0.0023 (13)
C20	0.0498 (15)	0.0497 (16)	0.0446 (14)	-0.0053 (13)	-0.0014 (12)	0.0051 (13)
C21	0.0516 (16)	0.0559 (17)	0.0497 (16)	0.0024 (14)	0.0067 (12)	-0.0002 (13)
C22	0.0516 (16)	0.0417 (15)	0.0575 (16)	0.0052 (12)	-0.0014 (13)	0.0000 (13)
C23	0.0591 (18)	0.075 (2)	0.0546 (18)	0.0052 (14)	0.0030 (14)	0.0043 (16)

Geometric parameters (\AA , $^\circ$)

N1—C16	1.380 (2)	C10—C11	1.387 (3)
N1—C1	1.385 (2)	C11—C12	1.382 (3)
N1—C9	1.416 (2)	C11—H11	0.9300
N2—C16	1.314 (2)	C12—C13	1.371 (3)
N2—N3	1.379 (2)	C12—H12	0.9300
N3—C1	1.318 (3)	C13—C14	1.362 (3)
N4—C23	1.133 (3)	C13—H13	0.9300

C1—C2	1.426 (3)	C14—C15	1.377 (3)
C2—C3	1.398 (3)	C14—H14	0.9300
C2—C7	1.404 (3)	C15—H15	0.9300
C3—C4	1.372 (3)	C16—C17	1.467 (3)
C3—H3	0.9300	C17—C22	1.387 (3)
C4—C5	1.386 (3)	C17—C18	1.389 (3)
C4—H4	0.9300	C18—C19	1.379 (3)
C5—C6	1.374 (3)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.384 (3)
C6—C7	1.398 (3)	C19—H19	0.9300
C6—H6	0.9300	C20—C21	1.381 (3)
C7—C8	1.437 (3)	C20—C23	1.445 (3)
C8—C9	1.342 (3)	C21—C22	1.382 (3)
C8—H8	0.9300	C21—H21	0.9300
C9—C10	1.481 (3)	C22—H22	0.9300
C10—C15	1.384 (3)		
C16—N1—C1	104.23 (17)	C12—C11—H11	120.1
C16—N1—C9	133.97 (18)	C10—C11—H11	120.1
C1—N1—C9	121.67 (19)	C13—C12—C11	120.5 (2)
C16—N2—N3	108.54 (17)	C13—C12—H12	119.7
C1—N3—N2	107.01 (17)	C11—C12—H12	119.7
N3—C1—N1	110.4 (2)	C14—C13—C12	120.1 (2)
N3—C1—C2	128.7 (2)	C14—C13—H13	119.9
N1—C1—C2	120.8 (2)	C12—C13—H13	119.9
C3—C2—C7	119.7 (2)	C13—C14—C15	120.1 (2)
C3—C2—C1	122.7 (2)	C13—C14—H14	120.0
C7—C2—C1	117.6 (2)	C15—C14—H14	120.0
C4—C3—C2	120.4 (2)	C14—C15—C10	120.7 (2)
C4—C3—H3	119.8	C14—C15—H15	119.7
C2—C3—H3	119.8	C10—C15—H15	119.7
C3—C4—C5	119.7 (2)	N2—C16—N1	109.78 (18)
C3—C4—H4	120.2	N2—C16—C17	123.23 (19)
C5—C4—H4	120.2	N1—C16—C17	126.94 (19)
C6—C5—C4	121.2 (2)	C22—C17—C18	118.8 (2)
C6—C5—H5	119.4	C22—C17—C16	122.4 (2)
C4—C5—H5	119.4	C18—C17—C16	118.8 (2)
C5—C6—C7	119.9 (2)	C19—C18—C17	120.6 (2)
C5—C6—H6	120.0	C19—C18—H18	119.7
C7—C6—H6	120.0	C17—C18—H18	119.7
C6—C7—C2	119.1 (2)	C18—C19—C20	119.9 (2)
C6—C7—C8	122.1 (2)	C18—C19—H19	120.1
C2—C7—C8	118.6 (2)	C20—C19—H19	120.1
C9—C8—C7	124.0 (2)	C21—C20—C19	120.2 (2)
C9—C8—H8	118.0	C21—C20—C23	119.9 (2)
C7—C8—H8	118.0	C19—C20—C23	119.9 (2)
C8—C9—N1	116.90 (19)	C20—C21—C22	119.7 (2)
C8—C9—C10	122.32 (19)	C20—C21—H21	120.2
N1—C9—C10	120.61 (19)	C22—C21—H21	120.2
C15—C10—C11	118.9 (2)	C21—C22—C17	120.8 (2)

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C15—C10—C9	119.4 (2)	C21—C22—H22	119.6
C11—C10—C9	121.49 (19)	C17—C22—H22	119.6
C12—C11—C10	119.7 (2)	N4—C23—C20	179.2 (3)
C16—N2—N3—C1	0.5 (2)	N1—C9—C10—C15	-131.8 (2)
N2—N3—C1—N1	0.3 (2)	C8—C9—C10—C11	-121.8 (2)
N2—N3—C1—C2	-178.9 (2)	N1—C9—C10—C11	53.2 (3)
C16—N1—C1—N3	-0.9 (2)	C15—C10—C11—C12	1.0 (3)
C9—N1—C1—N3	175.46 (16)	C9—C10—C11—C12	176.0 (2)
C16—N1—C1—C2	178.40 (18)	C10—C11—C12—C13	-0.9 (3)
C9—N1—C1—C2	-5.2 (3)	C11—C12—C13—C14	-0.4 (4)
N3—C1—C2—C3	-2.5 (3)	C12—C13—C14—C15	1.4 (4)
N1—C1—C2—C3	178.35 (17)	C13—C14—C15—C10	-1.3 (4)
N3—C1—C2—C7	178.8 (2)	C11—C10—C15—C14	0.0 (3)
N1—C1—C2—C7	-0.4 (3)	C9—C10—C15—C14	-175.0 (2)
C7—C2—C3—C4	0.2 (3)	N3—N2—C16—N1	-1.0 (2)
C1—C2—C3—C4	-178.5 (2)	N3—N2—C16—C17	176.63 (18)
C2—C3—C4—C5	-0.8 (3)	C1—N1—C16—N2	1.2 (2)
C3—C4—C5—C6	0.4 (3)	C9—N1—C16—N2	-174.51 (19)
C4—C5—C6—C7	0.7 (3)	C1—N1—C16—C17	-176.38 (19)
C5—C6—C7—C2	-1.2 (3)	C9—N1—C16—C17	7.9 (4)
C5—C6—C7—C8	174.57 (19)	N2—C16—C17—C22	-120.5 (2)
C3—C2—C7—C6	0.8 (3)	N1—C16—C17—C22	56.7 (3)
C1—C2—C7—C6	179.55 (19)	N2—C16—C17—C18	57.8 (3)
C3—C2—C7—C8	-175.16 (18)	N1—C16—C17—C18	-125.0 (2)
C1—C2—C7—C8	3.6 (3)	C22—C17—C18—C19	-3.0 (3)
C6—C7—C8—C9	-177.2 (2)	C16—C17—C18—C19	178.6 (2)
C2—C7—C8—C9	-1.5 (3)	C17—C18—C19—C20	1.4 (3)
C7—C8—C9—N1	-3.9 (3)	C18—C19—C20—C21	0.7 (3)
C7—C8—C9—C10	171.32 (18)	C18—C19—C20—C23	-178.3 (2)
C16—N1—C9—C8	-177.6 (2)	C19—C20—C21—C22	-1.2 (3)
C1—N1—C9—C8	7.3 (3)	C23—C20—C21—C22	177.8 (2)
C16—N1—C9—C10	7.0 (3)	C20—C21—C22—C17	-0.4 (3)
C1—N1—C9—C10	-168.06 (17)	C18—C17—C22—C21	2.5 (3)
C8—C9—C10—C15	53.1 (3)	C16—C17—C22—C21	-179.2 (2)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11—H11 \cdots N3 ⁱ	0.93	2.50	3.418 (3)	170

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

Fig. 1

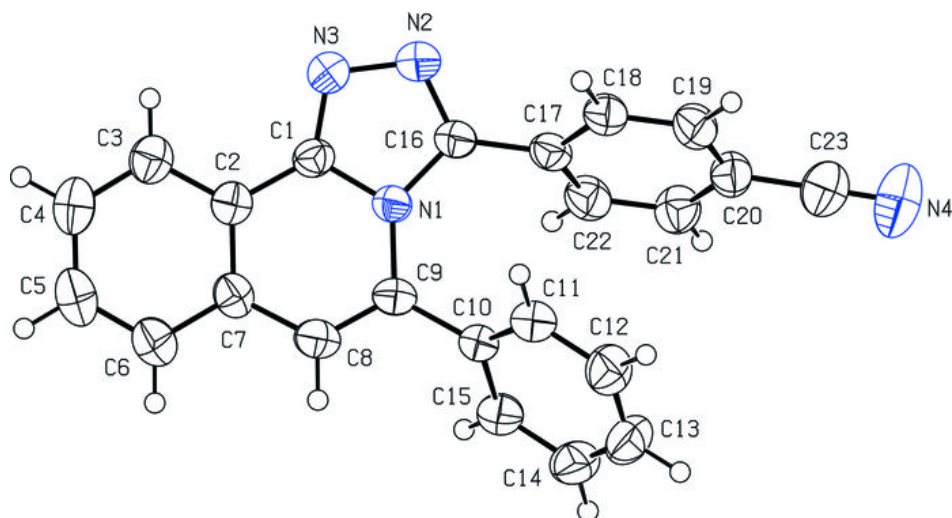


Fig. 2

