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A second monoclinic polymorph of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine

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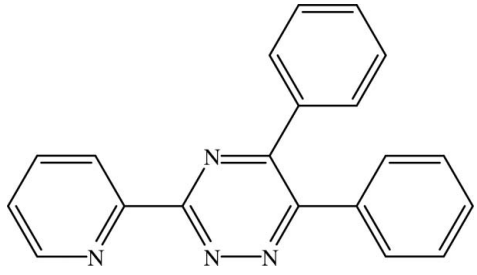
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.117; data-to-parameter ratio = 20.5.

A second monoclinic polymorph of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine, $C_{20}H_{14}N_4$, is reported. The unit-cell dimensions and the orientation of the pyridine ring with respect to the triazine ring are different from those of the previously reported monoclinic form [Eltayeb, Teoh, Ng, Fun & Ibrahim (2007). *Acta Cryst.* E**63**, o1041–o1042]. In the crystal structure, intermolecular C—H···N interactions connect the molecules into chains along the *c* axis. The crystal packing is also stabilized by C—H···π and π–π [centroid–centroid distance 3.5917 (9) Å] interactions. The crystal used was twinned and the ratio of the twin components refined to 0.726 (1)/0.274 (1).

Related literature

For bond-length data, see: Allen *et al.* (1987). For biological activities and applications of triazines, see: Almog *et al.* (1996); Croot & Hunter (2000); Mashly *et al.* (1999); Soudi *et al.* (2005). For related structures, see: Eltayeb, Guan & Yamin (2006); Eltayeb *et al.* (2007); Eltayeb, Teoh, Teh *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{14}N_4$
M_r = 310.35
Monoclinic, $P2_1/c$
a = 5.9729 (2) Å
b = 13.5580 (4) Å
c = 19.8855 (6) Å
β = 107.438 (1)°
V = 1536.33 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100.0 (1) K
0.57 × 0.16 × 0.16 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.954, T_{max} = 0.987
38187 measured reflections
4476 independent reflections
4101 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.117
S = 1.06
4476 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

*Cg*1 is the centroid of the C9–C14 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18···N1^{i}	0.93	2.56	3.477 (2)	167
C5—H5···*Cg*1^{ii}	0.93	2.63	3.522 (2)	160

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2435).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Almog, J., Hirshfeld, A., Glattstein, B., Sterling, J. & Goren, Z. (1996). *Anal. Chim. Acta*, **322**, 203–208.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Croot, P. L. & Hunter, K. A. (2000). *Anal. Chim. Acta*, **406**, 289–302.
Eltayeb, N. E., Guan, T. S. & Yamin, B. M. (2006). *Acta Cryst.* E**62**, m2284–m2286.
Eltayeb, N. E., Teoh, S. G., Ng, S.-L., Fun, H.-K. & Ibrahim, K. (2007). *Acta Cryst.* E**63**, o1041–o1042.

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Eltayeb, N. E., Teoh, S. G., Teh, J. B.-J., Fun, H.-K., Yamin, B. M. & Ibrahim, K. (2006). *Acta Cryst.* E**62**, m3336–m3337.
Mashly, M., Bayoumi, H. A. & Taha, A. (1999). *J. Serb. Chem. Soc.* **64**, 621–635.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Soudi, A. A., Marandi, F., Morsali, A., Kempe, R. & Hertle, I. (2005). *J. Coord. Chem.* **58**, 1631–1637.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2007). E**63**, o3792-o3793 [**doi:10.1107/S1600536807039463**]

A second monoclinic polymorph of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine

N. E. Eltayeb, S. G. Teoh, S. Chantrapromma, H.-K. Fun and K. Ibrahim

Comment

The 1,2,4-triazine compounds are well known natural products and show interesting biological, pharmacological and medicinal properties. The 3,5,6-trisubstituted-1,2,4-triazines are a principal class of N-donor heterocyclic ligands. Some can be active as blood platelet aggregation inhibitors and others exhibit antiviral activity, significant activity towards leukemia and ovarian cancer, and anti-HIV activity (Soudi *et al.*, 2005; Mashly *et al.*, 1999). Also 1,2,4-triazines have been used in analytical chemistry to determine the concentration of some trace metal ions (Almog *et al.*, 1996; Croot & Hunter 2000).

The crystal structure of the title compound was previously reported by Eltayeb *et al.* (2007) in the monoclinic space group $P2_1/c$, with with a = 11.5830 (3), b = 11.0381 (2), c = 11.9550 (3) Å, β = 94.127 (1)°, V = 1524.53 (6) Å^3 and Z = 4. In the present work, the compound crystallized again in the monoclinic space group $P2_1/c$, but with different cell parameters. The crystal used is found be twinned.

Bond lengths and angles in the title compound show normal values (Allen *et al.*, 1987), and are comparable to those observed in the other monoclinic polymorph (Eltayeb *et al.*, 2007) and related structures (Eltayeb, Teoh, Teh *et al.*, 2006; Eltayeb, Guan & Yamin, 2006). The C9–C14 and C15—C20 phenyl rings are attached to the triazine ring at atoms C2 and C3, with torsion angles C3—C2—C9—C14 = 35.9 (2)° [33.36 (14)° in the other polymorph (Eltayeb *et al.*, 2007)] and N3—C3—C15—C20 = 56.18 (18)° [51.09 (12)° in Eltayeb *et al.*, 2007]. The triazine ring in the present structure is essentially planar, the maximum deviation from planarity is 0.035 (1) Å for atom C3. The pyridine, C9–C14 and C15–C20 rings form dihedral angles of 7.69 (7)°, 34.41 (7)° and 57.39 (7)°, respectively, with the triazine ring. In the present structure atom N4 of the pyridine ring and N1 of the triazine ring are *cis* with respect to the C1—C4 bond [N1—C1—C4—N4 = 9.06 (19)°] while in the other monoclinic polymorph (Eltayeb *et al.*, 2007), the N4 and N3 atoms are *cis* with respect to the C1—C4 bond [N3—C1—C4—N4 = −1.04 (13)°].

In the crystal, the molecules are linked into chains along the *c* axis by C18—H18A···N1 hydrogen bonds (Fig. 2 and Table 1). In addition, C—H···π interactions (Table 1) involving the C9–C14 phenyl ring (centroid *Cg*1), and π-π stacking interactions involving the triazine ring (centroid *Cg*2) at (*x*, *y*, *z*) and the pyridine ring (centroid *Cg*3) at (*x* + 1, *y*,*z*) [*Cg*2···*Cg*3 =3.5917 (9) Å] are observed.

Experimental

The title compound was obtained unexpectedly during our attempt to prepare a Ir^{III} complex with 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine. A mixture of 5,6-diphenyl-3-(2-pyridyl)- 1,2,4-triazine (0.310 g, 1.0 mmol) and $IrCl_3$ (0.298 g, 1.0 mmol) in acetonitrile (20 ml) was refluxed for 2 h. The resulting dark-red solution was filtered and left to evaporate slowly at room temperature. Orange crystals suitable for X-ray diffraction were obtained after a few days.

Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The crystal was twinned and for a successful refinement the twin law (1 0 0/0 − 1 0/-2 0 − 1) was applied. The ratio of the twin components refined to 0.726 (1)/0.274 (1).

Figures

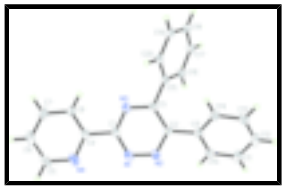

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering.

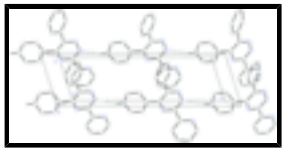

Fig. 2. The crystal packing of the title compound, viewed approximately along the *a* axis. Hydrogen bonds are shown as dashed lines.

5,6-Diphenyl-3-(2-pyridyl)-1,2,4-triazine

Crystal data

$C_{20}H_{14}N_4$	F_{000} = 648
M_r = 310.35	D_x = 1.342 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yb	Cell parameters from 4476 reflections
a = 5.9729 (2) Å	θ = 1.1–30.0º
b = 13.5580 (4) Å	μ = 0.08 mm^{-1}
c = 19.8855 (6) Å	*T* = 100.0 (1) K
β = 107.438 (1)º	Block, orange
V = 1536.33 (8) Å^3	0.57 × 0.16 × 0.16 mm
Z = 4	

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	4476 independent reflections
Radiation source: fine-focus sealed tube	4101 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 30.0º
T = 100.0(1) K	θ_{min} = 1.1º
ω scans	*h* = −8→8
Absorption correction: multi-scan (SADABS; Bruker, 2005)	*k* = −19→19

T_{min} = 0.954, T_{max} = 0.987
38187 measured reflections

l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.117
S = 1.06
4476 reflections
218 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.4643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: none

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.0885 (2)	0.63510 (9)	0.19330 (6)	0.0209 (2)
N2	0.2552 (2)	0.69821 (9)	0.18859 (6)	0.0196 (2)
N3	−0.1071 (2)	0.65178 (9)	0.07043 (6)	0.0200 (2)
N4	−0.2802 (3)	0.52978 (13)	0.21111 (8)	0.0375 (4)
C1	−0.0899 (2)	0.61748 (10)	0.13517 (8)	0.0190 (3)
C2	0.2460 (2)	0.73841 (9)	0.12619 (7)	0.0170 (3)
C3	0.0653 (2)	0.71036 (10)	0.06486 (7)	0.0174 (3)
C4	−0.2826 (2)	0.55369 (10)	0.14390 (8)	0.0195 (3)
C5	−0.4601 (3)	0.47228 (15)	0.21788 (10)	0.0378 (4)
H5	−0.4614	0.4535	0.2628	0.045*
C6	−0.6398 (3)	0.44113 (11)	0.16042 (10)	0.0304 (4)
H6	−0.7617	0.4026	0.1661	0.036*
C7	−0.6335 (3)	0.46882 (15)	0.09450 (10)	0.0373 (4)
H7	−0.7528	0.4481	0.0551	0.045*
C8	−0.4566 (3)	0.52592 (13)	0.08537 (8)	0.0287 (3)

H8	−0.4550	0.5452	0.0406	0.034*
C9	0.4333 (3)	0.81146 (10)	0.12891 (7)	0.0183 (3)
C10	0.6530 (3)	0.79836 (10)	0.17869 (8)	0.0197 (3)
H10	0.6800	0.7434	0.2080	0.024*
C11	0.8312 (3)	0.86651 (11)	0.18478 (9)	0.0262 (3)
H11	0.9775	0.8565	0.2175	0.031*
C12	0.7913 (3)	0.94958 (12)	0.14202 (10)	0.0314 (3)
H12	0.9112	0.9949	0.1457	0.038*
C13	0.5719 (3)	0.96479 (11)	0.09374 (9)	0.0291 (3)
H13	0.5441	1.0213	0.0659	0.035*
C14	0.3935 (3)	0.89615 (11)	0.08669 (8)	0.0231 (3)
H14	0.2475	0.9065	0.0539	0.028*
C15	0.0542 (2)	0.74154 (10)	−0.00777 (7)	0.0177 (3)
C16	0.2385 (3)	0.72039 (11)	−0.03508 (8)	0.0217 (3)
H16	0.3721	0.6883	−0.0075	0.026*
C17	0.2210 (3)	0.74768 (11)	−0.10402 (8)	0.0238 (3)
H17	0.3423	0.7328	−0.1227	0.029*
C18	0.0233 (3)	0.79704 (11)	−0.14501 (8)	0.0239 (3)
H18	0.0135	0.8160	−0.1908	0.029*
C19	−0.1599 (3)	0.81814 (12)	−0.11768 (8)	0.0257 (3)
H19	−0.2919	0.8515	−0.1450	0.031*
C20	−0.1459 (3)	0.78941 (11)	−0.04947 (8)	0.0225 (3)
H20	−0.2701	0.8021	−0.0316	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0226 (6)	0.0209 (5)	0.0229 (6)	0.0003 (5)	0.0121 (5)	0.0018 (5)
N2	0.0201 (6)	0.0209 (5)	0.0195 (5)	0.0005 (5)	0.0084 (5)	0.0008 (4)
N3	0.0193 (6)	0.0187 (5)	0.0230 (6)	−0.0011 (5)	0.0082 (5)	−0.0008 (4)
N4	0.0257 (7)	0.0520 (9)	0.0347 (8)	0.0001 (7)	0.0088 (6)	0.0220 (7)
C1	0.0205 (6)	0.0157 (6)	0.0245 (7)	0.0009 (5)	0.0124 (5)	−0.0002 (5)
C2	0.0183 (6)	0.0168 (6)	0.0178 (6)	0.0014 (5)	0.0084 (5)	−0.0014 (5)
C3	0.0183 (6)	0.0171 (6)	0.0181 (6)	0.0007 (5)	0.0078 (5)	−0.0006 (5)
C4	0.0198 (6)	0.0158 (6)	0.0262 (7)	0.0006 (5)	0.0116 (6)	0.0006 (5)
C5	0.0262 (8)	0.0565 (11)	0.0338 (9)	0.0057 (8)	0.0136 (7)	0.0265 (8)
C6	0.0296 (8)	0.0179 (7)	0.0505 (10)	−0.0031 (6)	0.0226 (8)	0.0000 (6)
C7	0.0288 (8)	0.0528 (11)	0.0334 (9)	−0.0189 (8)	0.0142 (7)	−0.0218 (8)
C8	0.0295 (8)	0.0419 (9)	0.0192 (6)	−0.0180 (7)	0.0142 (6)	−0.0141 (6)
C9	0.0216 (7)	0.0177 (6)	0.0175 (6)	−0.0016 (5)	0.0091 (5)	−0.0033 (5)
C10	0.0207 (6)	0.0173 (6)	0.0226 (7)	0.0006 (5)	0.0086 (5)	−0.0031 (5)
C11	0.0196 (7)	0.0234 (7)	0.0358 (8)	−0.0018 (5)	0.0085 (6)	−0.0058 (6)
C12	0.0282 (8)	0.0223 (7)	0.0465 (10)	−0.0077 (6)	0.0157 (8)	−0.0033 (6)
C13	0.0396 (9)	0.0193 (7)	0.0306 (8)	−0.0047 (6)	0.0137 (7)	0.0009 (6)
C14	0.0279 (7)	0.0212 (6)	0.0197 (6)	−0.0018 (6)	0.0064 (6)	−0.0006 (5)
C15	0.0190 (6)	0.0182 (6)	0.0161 (6)	−0.0030 (5)	0.0056 (5)	−0.0008 (5)
C16	0.0205 (7)	0.0254 (7)	0.0194 (6)	0.0009 (5)	0.0066 (5)	0.0004 (5)
C17	0.0252 (7)	0.0284 (7)	0.0198 (7)	−0.0034 (6)	0.0100 (6)	−0.0019 (5)

C18	0.0283 (8)	0.0254 (7)	0.0171 (6)	−0.0071 (6)	0.0057 (6)	0.0009 (5)
C19	0.0221 (7)	0.0281 (7)	0.0237 (7)	−0.0015 (6)	0.0020 (6)	0.0050 (6)
C20	0.0184 (6)	0.0263 (7)	0.0231 (7)	−0.0006 (5)	0.0067 (5)	0.0021 (5)

Geometric parameters (Å, °)

N1—N2	1.3376 (17)	C10—C11	1.387 (2)
N1—C1	1.3381 (19)	C10—H10	0.93
N2—C2	1.3413 (18)	C11—C12	1.388 (2)
N3—C3	1.3311 (18)	C11—H11	0.93
N3—C1	1.3434 (18)	C12—C13	1.388 (3)
N4—C5	1.367 (2)	C12—H12	0.93
N4—C4	1.3711 (19)	C13—C14	1.390 (2)
C1—C4	1.4909 (19)	C13—H13	0.93
C2—C3	1.4169 (19)	C14—H14	0.93
C2—C9	1.4828 (19)	C15—C20	1.394 (2)
C3—C15	1.4872 (18)	C15—C16	1.396 (2)
C4—C8	1.361 (2)	C16—C17	1.393 (2)
C5—C6	1.379 (3)	C16—H16	0.93
C5—H5	0.93	C17—C18	1.389 (2)
C6—C7	1.375 (3)	C17—H17	0.93
C6—H6	0.93	C18—C19	1.390 (2)
C7—C8	1.365 (2)	C18—H18	0.93
C7—H7	0.93	C19—C20	1.389 (2)
C8—H8	0.93	C19—H19	0.93
C9—C10	1.398 (2)	C20—H20	0.93
C9—C14	1.4001 (19)		
N2—N1—C1	118.07 (12)	C11—C10—H10	119.7
N1—N2—C2	119.98 (12)	C9—C10—H10	119.7
C3—N3—C1	116.59 (12)	C10—C11—C12	120.03 (15)
C5—N4—C4	116.87 (15)	C10—C11—H11	120.0
N1—C1—N3	125.34 (13)	C12—C11—H11	120.0
N1—C1—C4	116.46 (12)	C11—C12—C13	119.83 (15)
N3—C1—C4	118.20 (13)	C11—C12—H12	120.1
N2—C2—C3	119.79 (12)	C13—C12—H12	120.1
N2—C2—C9	114.59 (12)	C12—C13—C14	120.44 (15)
C3—C2—C9	125.62 (12)	C12—C13—H13	119.8
N3—C3—C2	119.81 (12)	C14—C13—H13	119.8
N3—C3—C15	116.10 (12)	C13—C14—C9	120.09 (15)
C2—C3—C15	124.09 (12)	C13—C14—H14	120.0
C8—C4—N4	123.42 (14)	C9—C14—H14	120.0
C8—C4—C1	118.63 (13)	C20—C15—C16	120.00 (13)
N4—C4—C1	117.88 (14)	C20—C15—C3	119.41 (13)
N4—C5—C6	122.22 (15)	C16—C15—C3	120.56 (13)
N4—C5—H5	118.9	C17—C16—C15	119.53 (14)
C6—C5—H5	118.9	C17—C16—H16	120.2
C7—C6—C5	117.99 (15)	C15—C16—H16	120.2
C7—C6—H6	121.0	C18—C17—C16	120.34 (14)
C5—C6—H6	121.0	C18—C17—H17	119.8

C8—C7—C6	121.68 (16)	C16—C17—H17	119.8
C8—C7—H7	119.2	C17—C18—C19	120.02 (14)
C6—C7—H7	119.2	C17—C18—H18	120.0
C4—C8—C7	117.79 (15)	C19—C18—H18	120.0
C4—C8—H8	121.1	C20—C19—C18	119.99 (15)
C7—C8—H8	121.1	C20—C19—H19	120.0
C10—C9—C14	118.90 (13)	C18—C19—H19	120.0
C10—C9—C2	118.61 (12)	C19—C20—C15	120.10 (14)
C14—C9—C2	122.36 (13)	C19—C20—H20	119.9
C11—C10—C9	120.68 (13)	C15—C20—H20	119.9
C1—N1—N2—C2	−2.93 (19)	N2—C2—C9—C10	32.21 (17)
N2—N1—C1—N3	5.8 (2)	C3—C2—C9—C10	−148.35 (14)
N2—N1—C1—C4	−174.83 (11)	N2—C2—C9—C14	−143.56 (14)
C3—N3—C1—N1	−2.1 (2)	C3—C2—C9—C14	35.9 (2)
C3—N3—C1—C4	178.48 (11)	C14—C9—C10—C11	−1.9 (2)
N1—N2—C2—C3	−2.89 (19)	C2—C9—C10—C11	−177.85 (13)
N1—N2—C2—C9	176.59 (11)	C9—C10—C11—C12	1.1 (2)
C1—N3—C3—C2	−4.02 (19)	C10—C11—C12—C13	0.7 (2)
C1—N3—C3—C15	175.40 (12)	C11—C12—C13—C14	−1.6 (3)
N2—C2—C3—N3	6.56 (19)	C12—C13—C14—C9	0.7 (2)
C9—C2—C3—N3	−172.86 (12)	C10—C9—C14—C13	1.1 (2)
N2—C2—C3—C15	−172.81 (13)	C2—C9—C14—C13	176.81 (13)
C9—C2—C3—C15	7.8 (2)	N3—C3—C15—C20	56.18 (18)
C5—N4—C4—C8	2.2 (2)	C2—C3—C15—C20	−124.42 (15)
C5—N4—C4—C1	179.20 (14)	N3—C3—C15—C16	−121.70 (14)
N1—C1—C4—C8	−173.80 (14)	C2—C3—C15—C16	57.69 (19)
N3—C1—C4—C8	5.7 (2)	C20—C15—C16—C17	0.2 (2)
N1—C1—C4—N4	9.06 (19)	C3—C15—C16—C17	178.04 (14)
N3—C1—C4—N4	−171.47 (14)	C15—C16—C17—C18	1.1 (2)
C4—N4—C5—C6	−1.5 (3)	C16—C17—C18—C19	−1.0 (2)
N4—C5—C6—C7	0.6 (3)	C17—C18—C19—C20	−0.3 (2)
C5—C6—C7—C8	−0.4 (3)	C18—C19—C20—C15	1.6 (2)
N4—C4—C8—C7	−2.0 (3)	C16—C15—C20—C19	−1.5 (2)
C1—C4—C8—C7	−178.98 (15)	C3—C15—C20—C19	−179.37 (13)
C6—C7—C8—C4	1.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···N1^{i}	0.93	2.56	3.477 (2)	167
C5—H5···Cg1^{ii}	0.93	2.63	3.522 (2)	160

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

Fig. 1

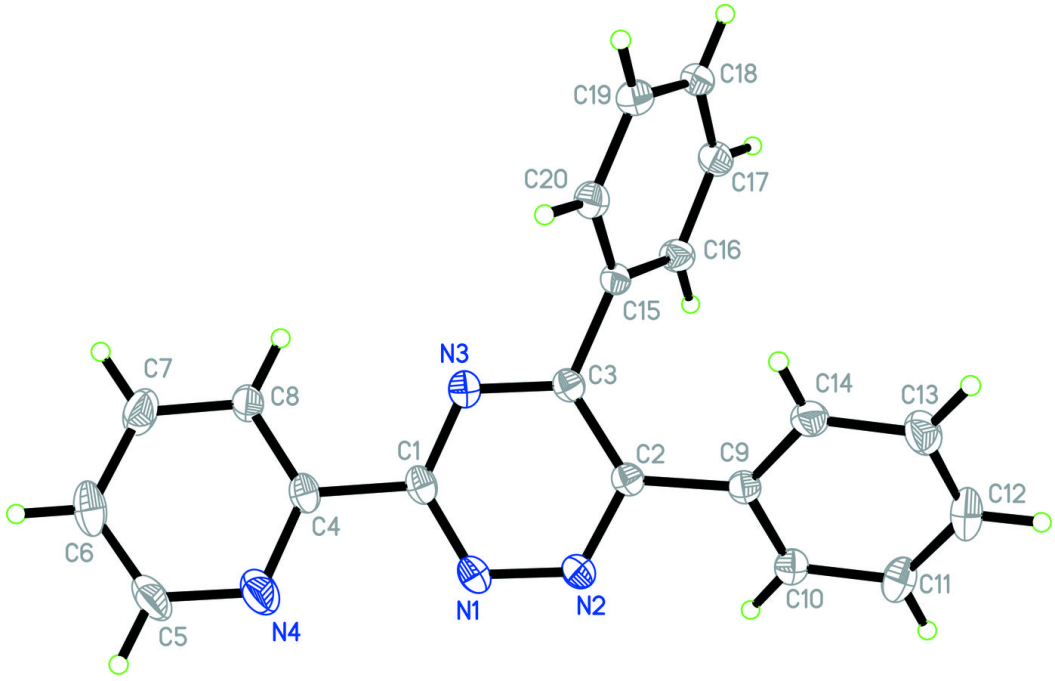
C18
C19
C17
C20
C16
C15
N3
C3
C7
C8
C14
C13
C1
C2
C9
C12
C4
C6
C10
C11
N1
N2
C5
N4

Fig. 2