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Crystal structure of 13-phenyl-2,3,4,13-tetrahydro-1*H*-indazolo[1,2-*b*]phthalazine-1,6,11-trione

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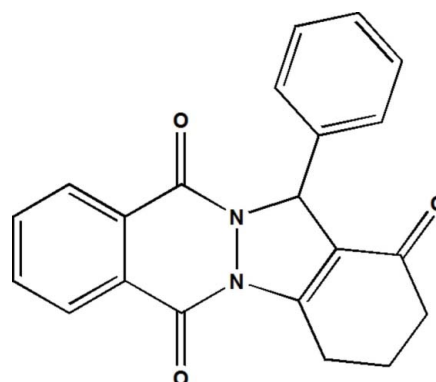
The title compound, C₂₁H₁₆N₂O₃, consists of an indazolone moiety, bearing a phenyl group, fused to a phthalazine ring system (r.m.s. deviation = 0.018 Å). The phenyl ring is almost normal to the mean plane of the five-membered ring of the indazolone moiety, making a dihedral angle of 89.64 (7)°. The six-membered ring of the indazolone moiety has an envelope conformation, with the central methylene C atom as the flap. In the crystal, molecules are linked *via* C—H...O hydrogen bonds, forming slabs parallel to the *bc* plane. The slabs are linked *via* C—H...π and π–π interactions [the shortest inter-centroid distance involving rings of pyrazolophthalazine moieties is 3.6430 (8) Å], forming a three-dimensional structure.

Keywords: crystal structure; indazolo; phthalazine-trione; C—H...O hydrogen bonds; π–π interactions.

CCDC reference: 1440831

1. Related literature

For application of phthalazine derivatives see: Mosaddegh & Hassankhani (2011); Hasaninejed *et al.* (2012); Keshipour *et al.* (2012). For the synthesis of this class of compounds, see: Carling *et al.* (2004); Cashman & Ghirmai (2009); Hall *et al.* (1992, 2001); Bouraiou *et al.* (2015); Nomoto *et al.* (1990). For the synthesis of the title compound, see: Bouraiou *et al.* (2015); Khurana & Magoo (2009); Nagarapu *et al.* (2009).



2. Experimental

2.1. Crystal data

C₂₁H₁₆N₂O₃
M_r = 344.36
 Monoclinic, *P*2₁/*c*
a = 8.9028 (2) Å
b = 11.4507 (3) Å
c = 17.0274 (4) Å
 β = 104.618 (1)°
V = 1679.64 (7) Å³
Z = 4
 Mo *K*α radiation
 μ = 0.09 mm⁻¹
T = 295 K
 0.13 × 0.09 × 0.05 mm

2.2. Data collection

Bruker APEXII diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2011)
T_{min} = 0.957, *T_{max}* = 0.986
 4873 measured reflections
 4873 independent reflections
 3617 reflections with *I* > 2σ(*I*)

2.3. Refinement

R[*F*² > 2σ(*F*²)] = 0.054
wR(*F*²) = 0.182
S = 1.12
 4873 reflections
 235 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max}$ = 0.6 e Å⁻³
 $\Delta\rho_{\min}$ = -0.28 e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

*Cg*3 is the centroid of the C2–C7 ring.

<i>D</i> — <i>H</i> ... <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> — <i>H</i> ... <i>A</i>
C5—H5...O2 ⁱ	0.93	2.59	3.488 (2)	163
C9—H9...O3 ⁱⁱ	0.98	2.54	3.501 (2)	165
C18—H18... <i>Cg</i> 3 ⁱⁱⁱ	0.93	2.68	3.552 (2)	156

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

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINTE* (Bruker, 2011); data reduction: *SAINTE*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5255).

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supporting information

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Crystal structure of 13-phenyl-2,3,4,13-tetrahydro-1*H*-indazolo[1,2-*b*]phthalazine-1,6,11-trione

Esma Lamera, Saida Benzerka, Abdelmalek Bouraiou, Sofiane Bouacida, Hocine Merazig, Aissa Chibani, Marc Le Borgne and Zouhair Bouaziz

S1. Comments

Phthalazine derivatives have been reported to act as anticonvulsants (Carling *et al.* 2004), potential inhibitors of serotonin reuptake (Cashman & Ghirmai, 2009), anti-proliferative agents against different human and murine tumor cells (Hall *et al.*, 1992, 2001) and vasorelaxant agents (Nomoto *et al.* 1990). Therefore, a number of synthetic methods have been developed in recent years to uncover a variety of new reagents for the synthesis of phthalazine derivatives (Mosaddegh & Hassankhani, 2011; Hasaninejed *et al.*, 2012; Keshipour *et al.*, 2012). In previous work, we have reported the synthesis and structure heterocyclic compounds bearing a phthalazine unit (Bouraiou *et al.*, 2015). Herein, we describe the synthesis and crystal structure of the title indazolo phthalazine-trione derivative, resulting from the reaction of phthalhydrazide, cyclohexa-1,3-dione and benzaldehyde in the presence of catalytic amounts of sulfuric acid.

The title compound, Fig. 1, consists of an indazolone moiety, bearing a phenyl group, fused to a phthalazine ring system [r.m.s. deviation = 0.018 Å]. The phenyl ring (C16—C21) is almost normal to the mean plane of the five-membered ring (N1/N2/C9/C10/C15) of the indazolone moiety with a dihedral angle of 89.64 (7)°. The six-membered ring of the indazolone moiety (C10—C15) has an envelope conformation with the central methylene C atom, C13, as the flap.

In the crystal, molecules are linked *via* C—H···O hydrogen bonds forming slabs parallel to the *bc* plane (Table 1 and Fig. 2). The slabs are linked *via* C—H··· π (Table 1) and slipped parallel π - π interactions [the shortest inter-centroid distance involves $Cg2\cdots Cg3^i = 3.6430$ (8) Å; $Cg2$ and $Cg3$ are the centroids of rings (N1/N2/C1/C2/C7/C8) and (C2—C7), respectively; inter-planar distance = 3.457 (5); slippage = 1.07 Å; symmetry code: (i) $-x + 1, -y, -z$], forming a three-dimensional structure.

S2. Synthesis and crystallization

The title compound was synthesized in accordance with established methods (Khurana & Magoo, 2009; Bouraiou *et al.*, 2015). Spectroscopic results and physical properties are in agreement with literature reports (Nagarapu *et al.*, 2009). The solid obtained, was recrystallized in a hot $\text{CHCl}_3/\text{EtOAc}/\text{EtOH}$ (1:1:1) mixture giving yellow crystals of the title compound. MS (ES-API): m/z [$M+H$] $^+$ = 345.1; $^1\text{H-NMR}$ δ (p.p.m.) (250 MHz, CDCl_3): 8.35–8.23 (m, 2H), 7.88–7.84 (m, 2H), 7.32–7.30 (m, 5H), 6.46 (s, 1H), 3.63–3.30 (m, 2H), 2.51–2.46 (m, 2H), 2.32–2.22 (m, 2H); $^{13}\text{C-NMR}$ δ (p.p.m.) (62.9 MHz, CDCl_3): 192.6, 156.1, 154.3, 152.3, 136.4, 134.6, 133.6, 129.1, 129.0, 128.7, 128.0, 127.8, 127.2, 119.7, 65.0, 37.0, 24.6, 22.3.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms were located in difference Fourier maps but introduced in calculated positions and refined as riding atoms: C—H = 0.93–0.98 Å with

$$U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}).$$

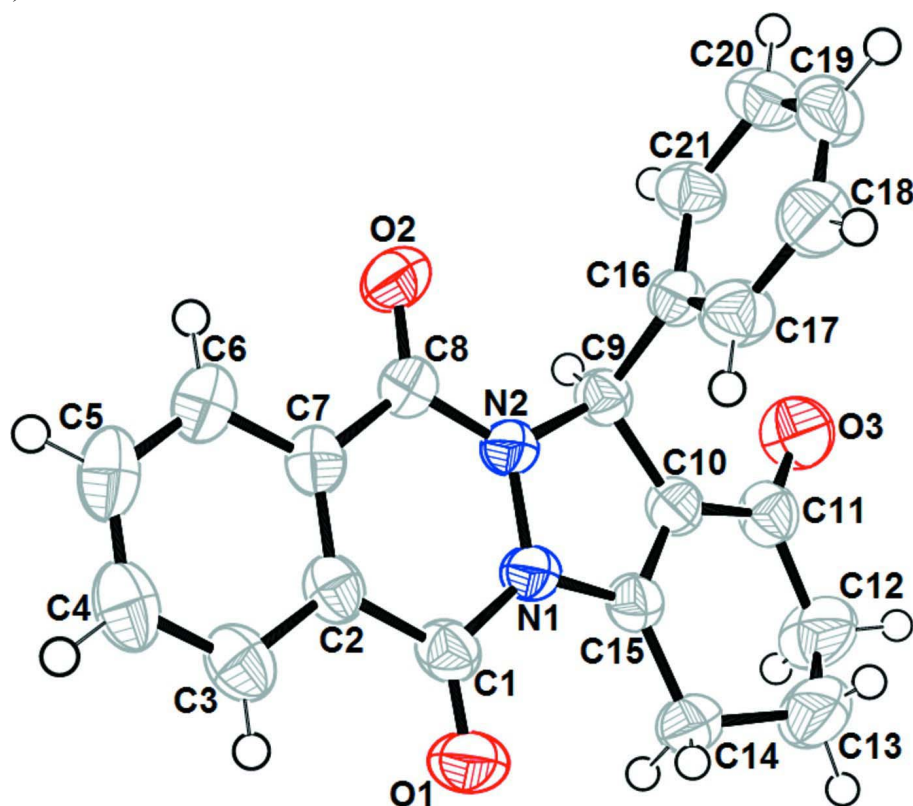


Figure 1

The molecule structure of the title compound, with atom labelling. Displacement are drawn at the 50% probability level.

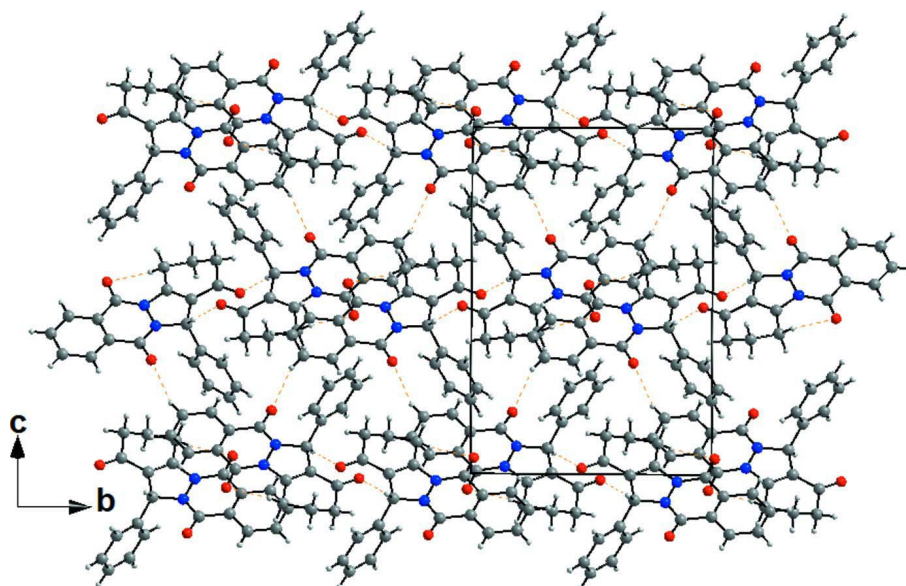


Figure 2

A view along the *a* axis of the crystal packing of the title compound, showing the C—H...O hydrogen bonds as dashed lines (see Table 1).

13-Phenyl-2,3,4,13-tetrahydro-1*H*-indazolo[1,2-*b*]phthalazine-1,6,11-trione

Crystal data

C₂₁H₁₆N₂O₃ $M_r = 344.36$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 8.9028$ (2) Å $b = 11.4507$ (3) Å $c = 17.0274$ (4) Å $\beta = 104.618$ (1)° $V = 1679.64$ (7) Å³ $Z = 4$ $F(000) = 720$ $D_x = 1.362$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4002 reflections

 $\theta = 3.0$ – 30.5 ° $\mu = 0.09$ mm⁻¹ $T = 295$ K

Prism, yellow

 $0.13 \times 0.09 \times 0.05$ mm

Data collection

Bruker APEXII
diffractometer

Radiation source: Enraf Nonius FR590

Graphite monochromator

CCD rotation images, thick slices scans

Absorption correction: multi-scan

(SADABS; Bruker, 2011)

 $T_{\min} = 0.957$, $T_{\max} = 0.986$

4873 measured reflections

4873 independent reflections

3617 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0$ $\theta_{\max} = 30.6$ °, $\theta_{\min} = 3.4$ ° $h = -12$ → 12 $k = 0$ → 16 $l = 0$ → 23

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.054$ $wR(F^2) = 0.182$ $S = 1.12$

4873 reflections

235 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.1115P)^2 + 0.0058P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.6$ e Å⁻³ $\Delta\rho_{\min} = -0.28$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.75069 (15)	0.02395 (11)	0.00764 (7)	0.0373 (3)
C2	0.68676 (14)	-0.05024 (11)	0.06179 (7)	0.0350 (3)
C3	0.69309 (16)	-0.17117 (12)	0.05347 (9)	0.0452 (3)
H3	0.7353	-0.2031	0.0136	0.054*

C4	0.63708 (18)	-0.24340 (13)	0.10405 (10)	0.0519 (4)
H4	0.6422	-0.324	0.0986	0.062*
C5	0.57284 (17)	-0.19596 (15)	0.16328 (10)	0.0525 (4)
H5	0.5359	-0.245	0.1977	0.063*
C6	0.56360 (16)	-0.07659 (14)	0.17128 (9)	0.0455 (3)
H6	0.5189	-0.0454	0.2105	0.055*
C7	0.62114 (13)	-0.00234 (12)	0.12069 (7)	0.0359 (3)
C8	0.60888 (14)	0.12553 (12)	0.12975 (7)	0.0369 (3)
C9	0.66558 (13)	0.31891 (11)	0.07410 (7)	0.0332 (3)
H9	0.5574	0.3454	0.0611	0.04*
C10	0.73305 (14)	0.33728 (11)	0.00262 (7)	0.0350 (3)
C11	0.74291 (16)	0.44774 (12)	-0.03792 (8)	0.0425 (3)
C12	0.8090 (2)	0.43883 (17)	-0.11124 (11)	0.0664 (5)
H12A	0.7242	0.4281	-0.1592	0.08*
H12B	0.8599	0.5119	-0.1175	0.08*
C13	0.9230 (3)	0.34114 (17)	-0.10670 (12)	0.0689 (5)
H13A	1.0152	0.358	-0.0639	0.083*
H13B	0.9534	0.3375	-0.1575	0.083*
C14	0.85967 (17)	0.22277 (14)	-0.09042 (8)	0.0464 (3)
H14A	0.7873	0.1942	-0.1392	0.056*
H14B	0.9439	0.167	-0.0747	0.056*
C15	0.77933 (14)	0.23569 (11)	-0.02380 (7)	0.0347 (3)
C16	0.75871 (13)	0.37878 (11)	0.15078 (7)	0.0329 (3)
C17	0.91360 (15)	0.35115 (14)	0.18289 (8)	0.0455 (3)
H17	0.9599	0.2926	0.1593	0.055*
C18	1.00001 (17)	0.41101 (16)	0.25044 (8)	0.0532 (4)
H18	1.1036	0.3916	0.2723	0.064*
C19	0.93283 (19)	0.49868 (14)	0.28486 (8)	0.0504 (4)
H19	0.9917	0.5398	0.3291	0.06*
C20	0.7781 (2)	0.52582 (13)	0.25386 (8)	0.0510 (4)
H20	0.7319	0.5841	0.2778	0.061*
C21	0.69169 (16)	0.46548 (12)	0.18660 (8)	0.0414 (3)
H21	0.5875	0.4839	0.1656	0.05*
N1	0.74174 (12)	0.14291 (9)	0.02082 (6)	0.0351 (2)
N2	0.67235 (12)	0.19043 (10)	0.07981 (6)	0.0355 (2)
O1	0.80699 (15)	-0.01280 (10)	-0.04590 (6)	0.0574 (3)
O2	0.54814 (13)	0.17285 (10)	0.17821 (6)	0.0539 (3)
O3	0.69339 (14)	0.53847 (10)	-0.01668 (7)	0.0591 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0465 (6)	0.0302 (6)	0.0353 (6)	0.0009 (5)	0.0105 (5)	0.0003 (5)
C2	0.0378 (6)	0.0291 (6)	0.0350 (6)	-0.0002 (5)	0.0031 (4)	0.0034 (4)
C3	0.0509 (7)	0.0333 (7)	0.0476 (7)	0.0004 (6)	0.0055 (6)	0.0010 (5)
C4	0.0562 (8)	0.0319 (7)	0.0630 (9)	-0.0035 (6)	0.0064 (7)	0.0072 (6)
C5	0.0506 (7)	0.0452 (8)	0.0599 (9)	-0.0093 (7)	0.0109 (6)	0.0166 (7)
C6	0.0442 (7)	0.0452 (8)	0.0483 (7)	-0.0045 (6)	0.0139 (5)	0.0077 (6)

C7	0.0345 (6)	0.0353 (7)	0.0359 (6)	-0.0030 (5)	0.0049 (4)	0.0035 (5)
C8	0.0389 (6)	0.0371 (7)	0.0362 (6)	-0.0031 (5)	0.0120 (4)	0.0007 (5)
C9	0.0361 (5)	0.0289 (6)	0.0347 (6)	0.0007 (5)	0.0093 (4)	-0.0005 (4)
C10	0.0397 (6)	0.0333 (7)	0.0314 (5)	-0.0019 (5)	0.0079 (4)	0.0008 (4)
C11	0.0483 (7)	0.0347 (7)	0.0437 (7)	-0.0015 (6)	0.0103 (5)	0.0054 (5)
C12	0.0946 (13)	0.0509 (10)	0.0660 (10)	0.0039 (9)	0.0433 (9)	0.0181 (8)
C13	0.0916 (13)	0.0537 (11)	0.0784 (11)	-0.0096 (9)	0.0530 (10)	0.0009 (9)
C14	0.0575 (8)	0.0435 (8)	0.0449 (7)	-0.0030 (7)	0.0254 (6)	-0.0026 (6)
C15	0.0395 (6)	0.0325 (6)	0.0325 (6)	-0.0035 (5)	0.0097 (4)	-0.0003 (5)
C16	0.0388 (6)	0.0304 (6)	0.0307 (5)	-0.0023 (5)	0.0110 (4)	0.0020 (4)
C17	0.0405 (6)	0.0532 (9)	0.0426 (6)	0.0032 (6)	0.0101 (5)	-0.0055 (6)
C18	0.0423 (7)	0.0717 (12)	0.0419 (7)	-0.0076 (7)	0.0037 (5)	0.0002 (7)
C19	0.0636 (9)	0.0497 (8)	0.0348 (6)	-0.0164 (7)	0.0068 (6)	-0.0031 (6)
C20	0.0734 (10)	0.0380 (7)	0.0417 (7)	0.0005 (7)	0.0145 (6)	-0.0052 (6)
C21	0.0491 (7)	0.0354 (7)	0.0399 (6)	0.0057 (6)	0.0115 (5)	0.0002 (5)
N1	0.0445 (5)	0.0300 (5)	0.0341 (5)	-0.0001 (4)	0.0159 (4)	-0.0015 (4)
N2	0.0449 (5)	0.0295 (5)	0.0362 (5)	-0.0021 (4)	0.0178 (4)	-0.0020 (4)
O1	0.0895 (8)	0.0395 (6)	0.0544 (6)	0.0026 (6)	0.0389 (6)	-0.0047 (5)
O2	0.0670 (7)	0.0471 (7)	0.0603 (6)	-0.0031 (5)	0.0394 (5)	-0.0030 (5)
O3	0.0773 (8)	0.0356 (6)	0.0685 (7)	0.0087 (5)	0.0262 (6)	0.0081 (5)

Geometric parameters (Å, °)

C1—O1	1.2206 (16)	C11—C12	1.512 (2)
C1—N1	1.3861 (16)	C12—C13	1.499 (3)
C1—C2	1.4700 (18)	C12—H12A	0.97
C2—C7	1.3942 (19)	C12—H12B	0.97
C2—C3	1.3945 (19)	C13—C14	1.520 (2)
C3—C4	1.375 (2)	C13—H13A	0.97
C3—H3	0.93	C13—H13B	0.97
C4—C5	1.389 (3)	C14—C15	1.4932 (19)
C4—H4	0.93	C14—H14A	0.97
C5—C6	1.378 (2)	C14—H14B	0.97
C5—H5	0.93	C15—N1	1.3951 (16)
C6—C7	1.3964 (18)	C16—C21	1.3775 (18)
C6—H6	0.93	C16—C17	1.3857 (18)
C7—C8	1.4793 (19)	C17—C18	1.3921 (19)
C8—O2	1.2215 (16)	C17—H17	0.93
C8—N2	1.3554 (16)	C18—C19	1.373 (2)
C9—N2	1.4746 (17)	C18—H18	0.93
C9—C10	1.5019 (17)	C19—C20	1.381 (2)
C9—C16	1.5217 (16)	C19—H19	0.93
C9—H9	0.98	C20—C21	1.3915 (19)
C10—C15	1.3487 (18)	C20—H20	0.93
C10—C11	1.4541 (18)	C21—H21	0.93
C11—O3	1.2187 (18)	N1—N2	1.4142 (14)
O1—C1—N1	120.73 (12)	H12A—C12—H12B	107.6

O1—C1—C2	124.48 (13)	C12—C13—C14	113.43 (16)
N1—C1—C2	114.78 (11)	C12—C13—H13A	108.9
C7—C2—C3	119.92 (13)	C14—C13—H13A	108.9
C7—C2—C1	121.51 (12)	C12—C13—H13B	108.9
C3—C2—C1	118.57 (13)	C14—C13—H13B	108.9
C4—C3—C2	120.21 (15)	H13A—C13—H13B	107.7
C4—C3—H3	119.9	C15—C14—C13	108.72 (12)
C2—C3—H3	119.9	C15—C14—H14A	109.9
C3—C4—C5	120.01 (15)	C13—C14—H14A	109.9
C3—C4—H4	120	C15—C14—H14B	109.9
C5—C4—H4	120	C13—C14—H14B	109.9
C6—C5—C4	120.36 (14)	H14A—C14—H14B	108.3
C6—C5—H5	119.8	C10—C15—N1	109.86 (11)
C4—C5—H5	119.8	C10—C15—C14	125.73 (12)
C5—C6—C7	120.17 (15)	N1—C15—C14	124.41 (12)
C5—C6—H6	119.9	C21—C16—C17	119.28 (12)
C7—C6—H6	119.9	C21—C16—C9	120.10 (11)
C2—C7—C6	119.32 (13)	C17—C16—C9	120.54 (11)
C2—C7—C8	121.32 (11)	C16—C17—C18	120.07 (14)
C6—C7—C8	119.35 (12)	C16—C17—H17	120
O2—C8—N2	120.42 (13)	C18—C17—H17	120
O2—C8—C7	124.50 (12)	C19—C18—C17	120.21 (13)
N2—C8—C7	115.08 (11)	C19—C18—H18	119.9
N2—C9—C10	100.09 (10)	C17—C18—H18	119.9
N2—C9—C16	112.86 (9)	C18—C19—C20	120.09 (13)
C10—C9—C16	112.92 (10)	C18—C19—H19	120
N2—C9—H9	110.2	C20—C19—H19	120
C10—C9—H9	110.2	C19—C20—C21	119.60 (14)
C16—C9—H9	110.2	C19—C20—H20	120.2
C15—C10—C11	122.13 (12)	C21—C20—H20	120.2
C15—C10—C9	111.58 (11)	C16—C21—C20	120.74 (13)
C11—C10—C9	126.22 (12)	C16—C21—H21	119.6
O3—C11—C10	122.07 (13)	C20—C21—H21	119.6
O3—C11—C12	123.22 (13)	C1—N1—C15	128.95 (11)
C10—C11—C12	114.58 (13)	C1—N1—N2	123.12 (11)
C13—C12—C11	114.02 (14)	C15—N1—N2	107.56 (10)
C13—C12—H12A	108.7	C8—N2—N1	124.10 (11)
C11—C12—H12A	108.7	C8—N2—C9	124.87 (11)
C13—C12—H12B	108.7	N1—N2—C9	110.79 (9)
C11—C12—H12B	108.7		

Hydrogen-bond geometry (Å, °)

Cg3 is the centroid of the C2–C7 ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C5—H5···O2 ⁱ	0.93	2.59	3.488 (2)	163

C9—H9···O3 ⁱⁱ	0.98	2.54	3.501 (2)	165
C18—H18···Cg3 ⁱⁱⁱ	0.93	2.68	3.552 (2)	156

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