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(*E*)-5-(4-Methylbenzylidene)-1-phenyl-4,5,6,7-tetrahydro-1*H*-indazol-4-one

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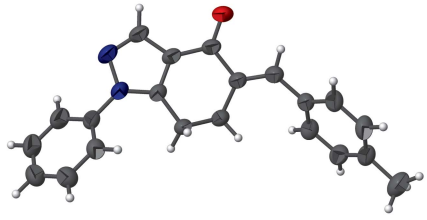
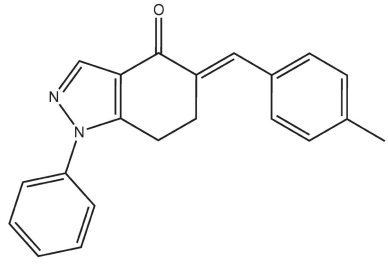
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{21}H_{18}N_2O$, the non-aromatic six-membered ring adopts a distorted envelope conformation with one of the methylene-C atoms being the flap atom. The dihedral angle between the phenyl and 4-tolyl rings is 75.3 (1)°. The 1,2-diazole ring forms dihedral angles of 41.9 (1) and 65.5 (1)° with the phenyl and 4-tolyl rings, respectively. In the crystal, stabilizing C—H···O, C—H···π and π–π interactions are evident. The calculated Hirshfeld surfaces highlight the prominent role of C—H···O interactions (8.6%), along with H···H (51.7%) and C···H/H···C (29.2%) surface contacts.

3D view



Chemical scheme



Structure description

Heterocyclic compounds have been investigated for a long while in view of their pharmaceutical and biological importance. 1,2-Diazole derivatives are found to possess antibacterial, anti-viral, anti-inflammatory, anti-depressant and anti-cancer activities (Popat *et al.*, 2003; Faisal *et al.*, 2019) because of their conformational freedom and exhibit intermolecular interactions of biological relevance. Owing to its medicinal interest and in a continuation of previous work, the crystal and molecular structures of another indazole derivative, namely, (*E*)-5-(4-methylbenzylidene)-1-phenyl-4,5,6,7-tetrahydro-1*H*-indazol-4-one, (I), is reported here.

The molecule of (I) and the recently reported 4-chlorobenzylidene derivative (II) (Meenatchi *et al.*, 2021) are isomorphous. The shorter *b*-axis lengths differ slightly between the isomorphous crystal structures, *i.e.* 8.7177 (5) Å for (I) and 8.6604 (5) Å for (II). In (I), the non-aromatic six-membered ring adopts a distorted envelope conformation with the methylene-C9 atom being the flap atom, Fig. 1. The heterocyclic five-

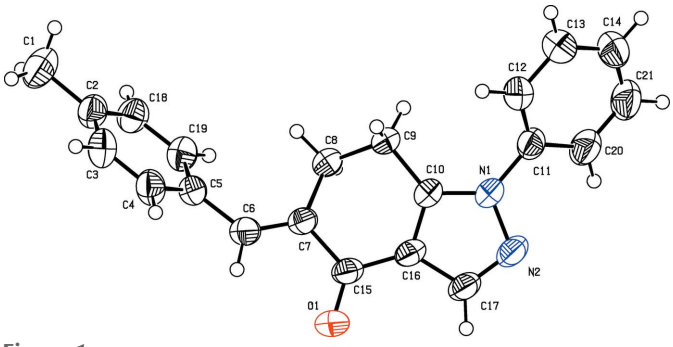


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids

membered ring forms dihedral angles of 41.9 (1) and 65.5 (1)° with the pendent N-bound phenyl and 4-tolyl rings, respectively. A weak intramolecular C6—H12···O1 interaction (Table 1) stabilizes the molecular structure.

The molecular packing features C—H···O, C—H···π and π–π interactions (Fig. 2). The C—H···O intermolecular interactions, *viz*., C12—H4···O1^{i} and C17—H5···O1^{ii}, lead, respectively, to two centrosymmetric ring $R_2^2(16)$ and $R_2^2(10)$ motifs (Bernstein *et al.*, 1995) (Fig. 3); see Table 1 for symmetry operations. These centrosymmetric dimers are connected through another C—H···O interaction, namely, C18—H8···O1^{iii}, leading to a chain *C*(8) motif along the *c*-axis direction of the unit cell (Fig. 4).

As a quantitative approach to analyse the intermolecular interactions, the Hirshfeld surfaces and two-dimensional (2-D) fingerprint plots were generated by employing the *Crystal Explorer* software (Wolff *et al.*, 2012). The Hirshfeld surface is colour-mapped with the normalized contact distance, d_{norm}, from red (distances shorter than the sum of the van der Waals radii) through white to blue (distances longer than the sum of the van der Waals radii). The different types of intermolecular interactions can be identified by colour coding the distances from the surface to the nearest atom exterior (d_e) or interior (d_i) plots to the surface. The 2-D fingerprint plots from the surface analysis and the d_{norm} surface were analysed for (I) to further explore the packing modes and intermolecular interactions. The 3-D Hirshfeld surfaces and 2-D fingerprint plots with percentage contributions are shown in Fig. 5. C···H/

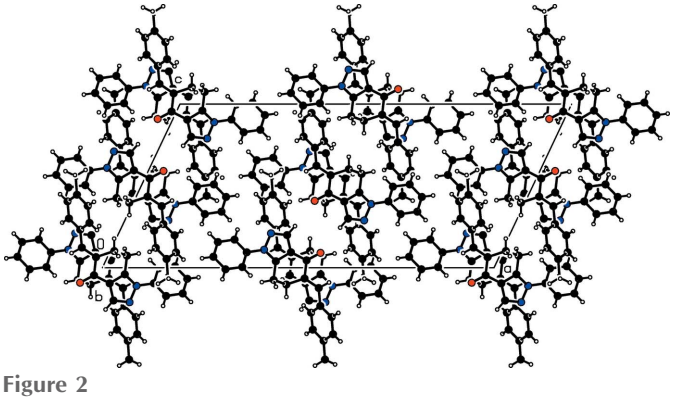


Figure 2
The molecular packing of (I), viewed down the *b* axis.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H12···O1	0.93	2.43	2.806 (2)	104
C12—H4···O1^{i}	0.93	2.52	3.312 (2)	143
C17—H5···O1^{ii}	0.93	2.60	3.5081 (19)	164
C18—H8···O1^{iii}	0.93	2.46	3.325 (2)	155

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

H···C contacts (with a pair of spikes in the fingerprint plot, 29.2%) and O···H/H···O interactions (sharp spikes, 8.6%) make a significant contribution to the overall contacts; the latter incorporate the notable C—H···O interactions. The H···H interactions contribute 51.7% with widely scattered points of high density showing a large proportion of hydrogen atoms in the molecular structure, indicating the importance of van der Waals contacts in the molecular packing. The N···H/H···N intermolecular contacts are identified as making a

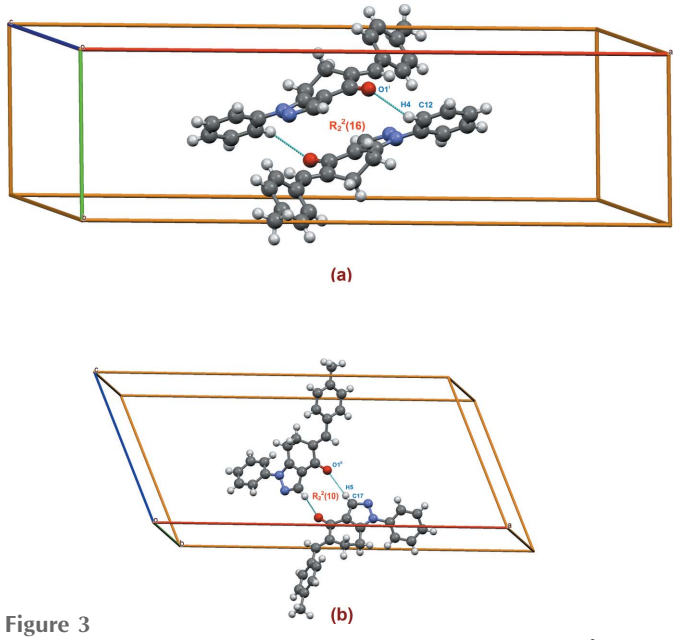


Figure 3
C—H···O interactions shown as dashed lines forming ring (*a*) $R_2^2(16)$ and (*b*) $R_2^2(10)$ motifs.

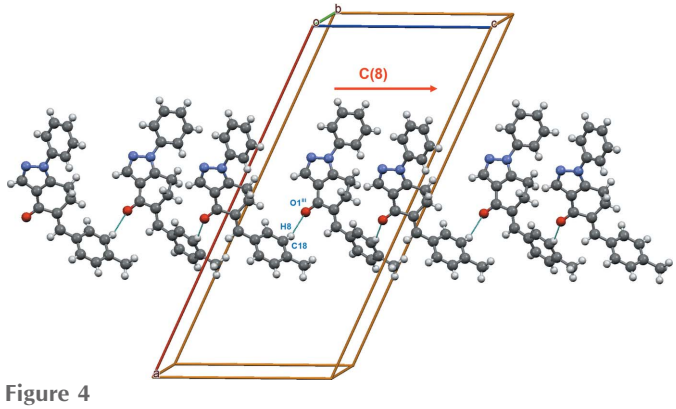


Figure 4
C—H···O interactions shown as dashed lines forming chain *C*(8) motif along *b* axis of the unit cell

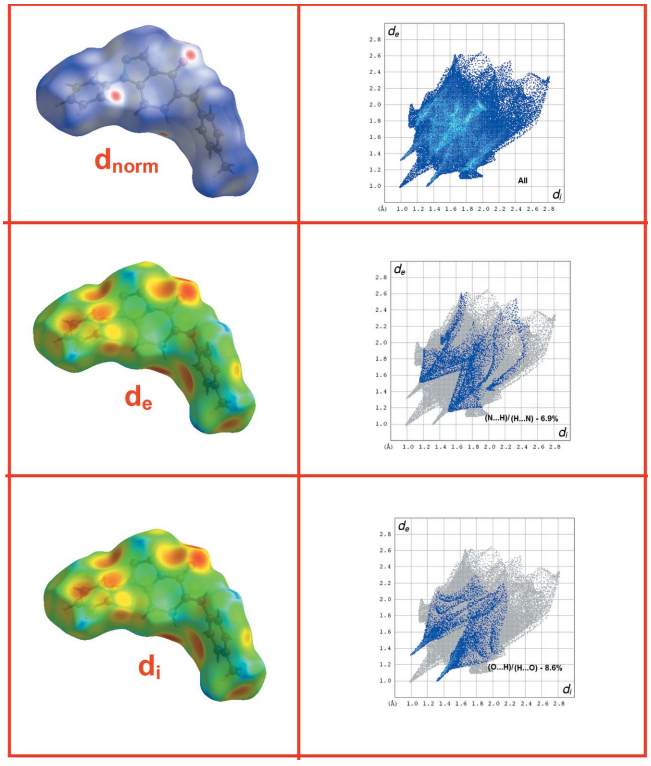


Figure 5
3-D Hirshfeld surfaces (showing d_{norm}, d_i and d_e) and 2-D fingerprint plots.

notable contribution to the total Hirshfeld surface comprising about 6.9%. However, the C—H···N intermolecular interactions are not prominent in the packing as the separations are greater than the van der Waals radii.

Synthesis and crystallization

A mixture of 1-phenyl-1,5,6,7-tetrahydro-4*H*-indazol-4-one (1 mmol) and 4-methylbenzaldehyde (1 mmol) was dissolved in ethanol followed by the addition of alcoholic NaOH. The mixture was stirred at room temperature for 1 h to afford (*E*)-5-(4-methylbenzylidene)-1-phenyl-1,5,6,7-tetrahydro-4*H*-indazol-4-ones as a precipitate, which was filtered, dried and recrystallized from ethanol: yield: 99%, m.p. 172–175°C.

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{18}N_2O$
M_r	314.37
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	30.3989 (15), 8.7177 (5), 14.0581 (7)
β (°)	115.367 (2)
V (Å^3)	3366.3 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.20 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker *SMART* APEXII CCD
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22457, 2948, 2557
R_{int}	0.048
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.126, 1.07
No. of reflections	2948
No. of parameters	219
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.18

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020) and *PLATON* (Spek, 2020).

Acknowledgements

JS and RV thank the management of The Madura College for their constant support and encouragement. The authors' contributions are as follows: Conceptualization, CSM; methodology, CSM, SA; investigation, CSM, RVP; synthesis, X-ray, analysis and validation, SA; writing (original draft), CSM; writing (review and editing of the manuscript), SRB; visualization, JS; resources, RVP, SRR; supervision, JS; project administration, SRB.

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full crystallographic data

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Crystal data

$C_{21}H_{18}N_2O$
M_r = 314.37
Monoclinic, *C*2/*c*
a = 30.3989 (15) Å
b = 8.7177 (5) Å
c = 14.0581 (7) Å
β = 115.367 (2)°
V = 3366.3 (3) Å^3
Z = 8
F(000) = 1328
D_x = 1.241 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3243 reflections
θ = 28.7–1.8°
μ = 0.08 mm^{-1}
T = 293 K
Block, colourless
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and *φ* scans
22457 measured reflections
2948 independent reflections
2557 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.0°, θ_{min} = 2.9°
h = −36→36
k = −10→10
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 1.07
2948 reflections
219 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
$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2 + 1.8343P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.075 (5)

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}
C1	0.67927 (8)	0.0162 (3)	1.06046 (15)	0.0789 (6)
H1	0.6816	−0.0935	1.0667	0.118*
H9	0.6614	0.0543	1.0977	0.118*
H10	0.7114	0.0599	1.0900	0.118*
C2	0.65323 (6)	0.0598 (2)	0.94602 (13)	0.0543 (4)
C3	0.66930 (6)	0.1813 (2)	0.90557 (14)	0.0586 (5)
H11	0.6970	0.2352	0.9496	0.070*
C4	0.64503 (6)	0.2237 (2)	0.80118 (14)	0.0550 (4)
H6	0.6572	0.3038	0.7758	0.066*
C5	0.60276 (5)	0.14887 (18)	0.73320 (12)	0.0450 (4)
C6	0.57687 (6)	0.20157 (19)	0.62334 (12)	0.0487 (4)
H12	0.5965	0.2260	0.5899	0.058*
C7	0.52919 (6)	0.21900 (18)	0.56538 (11)	0.0445 (4)
C8	0.48996 (6)	0.1884 (2)	0.60232 (12)	0.0516 (4)
H13	0.5052	0.1753	0.6781	0.062*
H14	0.4736	0.0931	0.5713	0.062*
C9	0.45177 (5)	0.3169 (2)	0.57388 (11)	0.0462 (4)
H15	0.4246	0.2838	0.5876	0.055*
H16	0.4660	0.4074	0.6160	0.055*
C10	0.43483 (5)	0.35272 (17)	0.45978 (11)	0.0416 (4)
C11	0.34983 (5)	0.45572 (19)	0.40541 (12)	0.0487 (4)
C12	0.35632 (6)	0.5344 (2)	0.49555 (13)	0.0541 (4)
H4	0.3875	0.5536	0.5471	0.065*
C13	0.31616 (7)	0.5847 (2)	0.50901 (16)	0.0657 (5)
H3	0.3205	0.6369	0.5701	0.079*
C14	0.27001 (7)	0.5582 (3)	0.43271 (17)	0.0761 (6)
H2	0.2431	0.5928	0.4417	0.091*
C15	0.51236 (6)	0.27563 (18)	0.45440 (11)	0.0449 (4)
C16	0.46258 (6)	0.32941 (18)	0.40502 (11)	0.0440 (4)
C17	0.43202 (6)	0.3710 (2)	0.30018 (12)	0.0518 (4)
H5	0.4413	0.3674	0.2453	0.062*
C18	0.61226 (6)	−0.01863 (19)	0.87812 (13)	0.0545 (4)
H8	0.6013	−0.1025	0.9029	0.065*
C19	0.58722 (6)	0.02523 (18)	0.77400 (13)	0.0509 (4)
H7	0.5595	−0.0287	0.7304	0.061*
C20	0.30333 (6)	0.4275 (3)	0.32794 (14)	0.0679 (5)
H18	0.2989	0.3743	0.2671	0.081*
C21	0.26374 (7)	0.4799 (3)	0.34264 (17)	0.0825 (7)
H17	0.2324	0.4620	0.2910	0.099*

N1	0.39101 (4)	0.40554 (15)	0.38972 (9)	0.0463 (3)
N2	0.38894 (5)	0.41551 (17)	0.28944 (10)	0.0550 (4)
O1	0.53899 (4)	0.27719 (16)	0.40893 (9)	0.0624 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0871 (14)	0.0832 (14)	0.0504 (11)	0.0112 (11)	0.0142 (10)	0.0108 (10)
C2	0.0548 (9)	0.0552 (10)	0.0472 (9)	0.0125 (7)	0.0163 (7)	0.0056 (7)
C3	0.0443 (8)	0.0577 (10)	0.0587 (10)	0.0017 (7)	0.0079 (7)	0.0034 (8)
C4	0.0442 (8)	0.0548 (10)	0.0624 (10)	0.0039 (7)	0.0192 (7)	0.0142 (8)
C5	0.0442 (8)	0.0470 (9)	0.0442 (8)	0.0097 (6)	0.0194 (6)	0.0042 (6)
C6	0.0527 (9)	0.0532 (9)	0.0453 (8)	0.0075 (7)	0.0259 (7)	0.0052 (7)
C7	0.0510 (8)	0.0484 (8)	0.0371 (7)	0.0075 (6)	0.0218 (6)	0.0038 (6)
C8	0.0522 (9)	0.0645 (10)	0.0409 (8)	0.0091 (7)	0.0226 (7)	0.0154 (7)
C9	0.0449 (8)	0.0614 (9)	0.0339 (7)	0.0044 (7)	0.0183 (6)	0.0071 (6)
C10	0.0443 (7)	0.0444 (8)	0.0329 (7)	−0.0007 (6)	0.0134 (6)	0.0012 (6)
C11	0.0432 (8)	0.0558 (9)	0.0430 (8)	0.0023 (7)	0.0146 (6)	0.0117 (7)
C12	0.0455 (8)	0.0617 (10)	0.0509 (9)	0.0024 (7)	0.0168 (7)	0.0010 (8)
C13	0.0602 (10)	0.0758 (13)	0.0659 (11)	0.0090 (9)	0.0317 (9)	0.0046 (9)
C14	0.0502 (10)	0.1054 (17)	0.0754 (14)	0.0144 (10)	0.0296 (10)	0.0224 (12)
C15	0.0550 (9)	0.0479 (9)	0.0366 (7)	0.0026 (7)	0.0244 (7)	−0.0001 (6)
C16	0.0547 (8)	0.0465 (8)	0.0313 (7)	0.0011 (6)	0.0191 (6)	0.0003 (6)
C17	0.0654 (10)	0.0582 (10)	0.0324 (8)	0.0072 (8)	0.0214 (7)	0.0027 (7)
C18	0.0589 (9)	0.0478 (9)	0.0540 (9)	0.0043 (7)	0.0217 (8)	0.0100 (7)
C19	0.0505 (9)	0.0457 (9)	0.0493 (9)	0.0013 (7)	0.0145 (7)	0.0004 (7)
C20	0.0513 (10)	0.0972 (15)	0.0440 (9)	−0.0042 (9)	0.0097 (7)	0.0053 (9)
C21	0.0429 (10)	0.128 (2)	0.0619 (12)	−0.0002 (11)	0.0088 (8)	0.0193 (13)
N1	0.0480 (7)	0.0545 (8)	0.0324 (6)	0.0029 (6)	0.0134 (5)	0.0035 (5)
N2	0.0639 (9)	0.0638 (9)	0.0313 (7)	0.0062 (7)	0.0146 (6)	0.0044 (6)
O1	0.0667 (8)	0.0851 (9)	0.0476 (7)	0.0143 (6)	0.0361 (6)	0.0098 (6)

Geometric parameters (Å, º)

C1—C2	1.506 (2)	C10—C16	1.379 (2)
C1—H1	0.9600	C11—C12	1.379 (2)
C1—H9	0.9600	C11—C20	1.388 (2)
C1—H10	0.9600	C11—N1	1.430 (2)
C2—C18	1.382 (2)	C12—C13	1.384 (2)
C2—C3	1.386 (3)	C12—H4	0.9300
C3—C4	1.381 (2)	C13—C14	1.372 (3)
C3—H11	0.9300	C13—H3	0.9300
C4—C5	1.392 (2)	C14—C21	1.378 (3)
C4—H6	0.9300	C14—H2	0.9300
C5—C19	1.395 (2)	C15—O1	1.2279 (18)
C5—C6	1.474 (2)	C15—C16	1.446 (2)
C6—C7	1.333 (2)	C16—C17	1.412 (2)
C6—H12	0.9300	C17—N2	1.311 (2)

C7—C15	1.502 (2)	C17—H5	0.9300
C7—C8	1.514 (2)	C18—C19	1.383 (2)
C8—C9	1.538 (2)	C18—H8	0.9300
C8—H13	0.9700	C19—H7	0.9300
C8—H14	0.9700	C20—C21	1.383 (3)
C9—C10	1.4925 (19)	C20—H18	0.9300
C9—H15	0.9700	C21—H17	0.9300
C9—H16	0.9700	N1—N2	1.3867 (17)
C10—N1	1.3535 (18)		

C2—C1—H1	109.5	C16—C10—C9	123.85 (13)
C2—C1—H9	109.5	C12—C11—C20	120.41 (16)
H1—C1—H9	109.5	C12—C11—N1	120.27 (13)
C2—C1—H10	109.5	C20—C11—N1	119.30 (15)
H1—C1—H10	109.5	C11—C12—C13	119.73 (16)
H9—C1—H10	109.5	C11—C12—H4	120.1
C18—C2—C3	117.79 (15)	C13—C12—H4	120.1
C18—C2—C1	121.21 (17)	C14—C13—C12	120.38 (19)
C3—C2—C1	120.99 (17)	C14—C13—H3	119.8
C4—C3—C2	121.26 (16)	C12—C13—H3	119.8
C4—C3—H11	119.4	C13—C14—C21	119.64 (18)
C2—C3—H11	119.4	C13—C14—H2	120.2
C3—C4—C5	121.32 (16)	C21—C14—H2	120.2
C3—C4—H6	119.3	O1—C15—C16	122.29 (13)
C5—C4—H6	119.3	O1—C15—C7	122.50 (14)
C4—C5—C19	117.09 (14)	C16—C15—C7	115.20 (12)
C4—C5—C6	119.64 (14)	C10—C16—C17	104.99 (13)
C19—C5—C6	123.27 (14)	C10—C16—C15	122.98 (13)
C7—C6—C5	128.94 (14)	C17—C16—C15	132.02 (14)
C7—C6—H12	115.5	N2—C17—C16	111.97 (14)
C5—C6—H12	115.5	N2—C17—H5	124.0
C6—C7—C15	118.02 (14)	C16—C17—H5	124.0
C6—C7—C8	125.46 (13)	C2—C18—C19	121.22 (16)
C15—C7—C8	116.51 (13)	C2—C18—H8	119.4
C7—C8—C9	113.58 (13)	C19—C18—H8	119.4
C7—C8—H13	108.8	C18—C19—C5	121.25 (15)
C9—C8—H13	108.8	C18—C19—H7	119.4
C7—C8—H14	108.8	C5—C19—H7	119.4
C9—C8—H14	108.8	C21—C20—C11	118.89 (19)
H13—C8—H14	107.7	C21—C20—H18	120.6
C10—C9—C8	107.83 (12)	C11—C20—H18	120.6
C10—C9—H15	110.1	C14—C21—C20	120.94 (18)
C8—C9—H15	110.1	C14—C21—H17	119.5
C10—C9—H16	110.1	C20—C21—H17	119.5
C8—C9—H16	110.1	C10—N1—N2	111.28 (12)
H15—C9—H16	108.5	C10—N1—C11	130.21 (12)
N1—C10—C16	106.89 (12)	N2—N1—C11	118.44 (12)
N1—C10—C9	129.20 (13)	C17—N2—N1	104.86 (12)

C18—C2—C3—C4	0.6 (3)	O1—C15—C16—C10	−168.78 (15)
C1—C2—C3—C4	−178.75 (18)	C7—C15—C16—C10	10.8 (2)
C2—C3—C4—C5	1.8 (3)	O1—C15—C16—C17	10.0 (3)
C3—C4—C5—C19	−2.7 (2)	C7—C15—C16—C17	−170.40 (16)
C3—C4—C5—C6	177.62 (15)	C10—C16—C17—N2	−0.38 (19)
C4—C5—C6—C7	−137.43 (18)	C15—C16—C17—N2	−179.36 (16)
C19—C5—C6—C7	42.9 (3)	C3—C2—C18—C19	−1.9 (3)
C5—C6—C7—C15	179.80 (15)	C1—C2—C18—C19	177.42 (17)
C5—C6—C7—C8	0.7 (3)	C2—C18—C19—C5	0.9 (3)
C6—C7—C8—C9	133.31 (17)	C4—C5—C19—C18	1.3 (2)
C15—C7—C8—C9	−45.8 (2)	C6—C5—C19—C18	−178.96 (15)
C7—C8—C9—C10	49.38 (18)	C12—C11—C20—C21	0.1 (3)
C8—C9—C10—N1	150.39 (16)	N1—C11—C20—C21	−178.39 (18)
C8—C9—C10—C16	−26.6 (2)	C13—C14—C21—C20	0.0 (4)
C20—C11—C12—C13	0.4 (3)	C11—C20—C21—C14	−0.3 (3)
N1—C11—C12—C13	178.88 (16)	C16—C10—N1—N2	0.89 (17)
C11—C12—C13—C14	−0.7 (3)	C9—C10—N1—N2	−176.49 (15)
C12—C13—C14—C21	0.5 (3)	C16—C10—N1—C11	−176.18 (15)
C6—C7—C15—O1	14.8 (2)	C9—C10—N1—C11	6.4 (3)
C8—C7—C15—O1	−166.01 (16)	C12—C11—N1—C10	36.0 (2)
C6—C7—C15—C16	−164.78 (15)	C20—C11—N1—C10	−145.48 (17)
C8—C7—C15—C16	14.4 (2)	C12—C11—N1—N2	−140.90 (16)
N1—C10—C16—C17	−0.32 (17)	C20—C11—N1—N2	37.6 (2)
C9—C10—C16—C17	177.24 (15)	C16—C17—N2—N1	0.89 (19)
N1—C10—C16—C15	178.78 (14)	C10—N1—N2—C17	−1.10 (18)
C9—C10—C16—C15	−3.7 (2)	C11—N1—N2—C17	176.35 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H12···O1	0.93	2.43	2.806 (2)	104
C12—H4···O1^{i}	0.93	2.52	3.312 (2)	143
C17—H5···O1^{ii}	0.93	2.60	3.5081 (19)	164
C18—H8···O1^{iii}	0.93	2.46	3.325 (2)	155

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