(E)-5-(4-Chlorobenzylidene)-1-phenyl-4,5,6,7-tetrahydro-1H-indazol-4-one: crystal structure and Hirshfeld surface analysis

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In the title compound, C20H15ClN2O, the non-aromatic six-membered ring adopts a distorted envelope conformation with methylene-C atom nearest to the five-membered ring being the flap atom. The dihedral angle between the phenyl and chlorobenzene rings is 74.5 (1). The heterocyclic ring forms dihedral angles of 37.9 (1) and 64.3 (1)° with the phenyl and chlorobenzene rings, respectively. In the crystal, weak C—H···O interactions feature predominantly within the three-dimensional architecture. The intermolecular interactions are further analysed with the calculation of the Hirshfeld surfaces highlighting the prominent role of C—H···O interactions, along with H···H (36.8%) and C···H/H···C (26.5%) contacts.

Structure description

Many heterocyclic compounds are studied for their biological and pharmacological activities. For example, 1,2-diazole derivatives are known to possess anti-depressant, antiviral, anti-inflammatory and anti-cancer activities (Popat et al., 2003; Faisal et al., 2019). The crystal and molecular structure of one such indazole derivative, namely, (E)-5-(4-chlorobenzylidene)-1-phenyl-4,5,6,7-tetrahydro-1H-indazol-4-one, is reported herein.

The non-aromatic six-membered ring adopts a distorted envelope conformation with the methylene-C10 atom being the flap atom, Fig. 1. The heterocyclic ring forms dihedral angles of 37.9 (1) and 64.3 (1)° with the phenyl and chlorobenzene rings, respectively. The
The molecular structure features a weak intramolecular interaction through C14—H14...O1 (Table 1).

The molecular packing features two ring motifs, viz., \(R^2_2(10)\) and \(R^2_2(16)\) (Bernstein et al., 1995), each around an inversion centre, through two C—H...O interactions, i.e., C7—H7...O1\(^\text{ii}\) and C5—H5...O1\(^\text{i}\), respectively, Fig. 2; for symmetry codes, refer to Table 1. The centrosymmetric dimers thus formed are connected through two C—H...X interactions, viz., C7—H17...O\(^\text{iii}\) and C2—H2...Cl\(^\text{iv}\), leading to chain C(8) and C(15) motifs, respectively. The first named interaction serves to connect the molecules along the along \([001]\) and the latter along \([101]\), Fig. 3. Clearly, the carbonyl-O1 atom plays a pivotal role in the supramolecular assembly.

The intermolecular interactions in the crystal state can be visualized through the calculation of the Hirshfeld surfaces and associated two-dimensional fingerprint plots. These were generated by Crystal Explorer (Wolff et al., 2012). The Hirshfeld surface is colour-mapped with the normalized contact distance, \(d_{\text{norm}}\), i.e., 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 distances from the surface to the nearest atom exterior (\(d_e\)) or interior (\(d_i\)) plots to the surface. The three-dimensional Hirshfeld surfaces and selected two-dimensional fingerprint plots (with percentage contributions) are given in Fig. 4.

The presence of spikes due to O...H/H...O interactions (8.6%) correspond to C—H...O intermolecular interactions, which feature predominantly within the crystalline assembly. The contribution of C...H/H...C contacts (26.5%), leading to a pair of well-defined wings, is also noteworthy. The H...H

### Table 1

| \(D—H\) | \(D—H\) | \(H—D\) | \(D—D\) | \(D—H\) |
|---------|---------|---------|---------|---------|
| C14—H14...O1 | 0.93 | 2.43 | 2.804 (3) | 104 |
| C5—H5...O1\(^\text{i}\) | 0.93 | 2.53 | 3.320 (3) | 143 |
| C7—H7...O1\(^\text{ii}\) | 0.93 | 2.59 | 3.493 (3) | 163 |
| C17—H17...O1\(^\text{iii}\) | 0.93 | 2.40 | 3.260 (3) | 154 |
| C2—H2...Cl\(^\text{iv}\) | 0.93 | 2.90 | 3.633 (3) | 157 |

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

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids

Figure 2

A view of the unit-cell contents viewed in projection down the \(b\)-axis.

Figure 3

Views of significant C—H...X interactions (X = O or Cl) shown as dashed lines forming (a) an \(R^2_1(10)\) ring motif, (b) an \(R^2_1(16)\) ring, (c) a C(8) chain motif and (d) a C(15) chain.

Figure 4

Hirshfeld three-dimensional surfaces (showing \(d_{\text{norm}}, d_e\) and \(d_i\)) and selected two-dimensional fingerprint plots
interactions contribute 36.8% with widely scattered points of high density, which is consistent with the large number of hydrogen atoms at the surface of the molecule. The Cl⋯H/H⋯Cl contacts also make a notable contribution to the total Hirshfeld surfaces, comprising about 12.9%. The large number of H⋯H, Cl⋯H/H⋯Cl, O⋯H/H⋯O interactions suggest that van der Waals interactions play a significant role in the packing in the crystal.

Synthesis and crystallization

A mixture of 1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one, (1 mmol) and 4-chlorobenzaldehyde (1 mmol) was dissolved in ethanol followed by the addition of NaOH. The resulting mixture was stirred at room temperature for 1 h to afford (E)-5-(4-chlorobenzylidene)-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-ones as the precipitate. This was filtered off and recrystallized from ethanol to afford colourless crystals; yield: 95%, m.p. 183–184°C.

Refinement

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

Acknowledgements

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Table 2

| Experimental details. |
|-----------------------|
| Crystal data |
| Chemical formula | C$_{20}$H$_{15}$ClN$_2$O |
| $M_r$ | 334.79 |
| Crystal system, space group | Monoclinic, C2/c |
| Temperature (K) | 293 |
| $a$, $b$, $c$ (Å) | 30.4808 (16), 8.6604 (5), 14.0457 (7) |
| $\beta$ (°) | 115.071 (2) |
| $V$ (Å$^3$) | 3358.4 (3) |
| $Z$ | 8 |
| Radiation type | Mo Kα |
| $\mu$ (mm$^{-1}$) | 0.24 |
| Crystal size (mm) | 0.22 × 0.20 × 0.16 |

Data collection

Diffractometer

Bruker SMART APEXII CCD

Absorption correction

–

No. of measured, independent and observed $|I > 2\sigma(I)|$ reflections

42189, 2949, 2353

$R_{int}$

0.056

$(\sin \theta/\lambda)_{max}$ (Å$^{-1}$)

0.606

Refinement

$R(F^2 > 2\sigma(F^2))$, $wR(F^2)$, $S$

0.051, 0.146, 1.12

No. of reflections

2949

No. of parameters

218

H-atom treatment

H-atom parameters constrained

$\Delta$ρ$_{max}$, $\Delta$ρ$_{min}$ (e Å$^{-3}$)

0.39, −0.44

Computer programs: APEX2 and SAINT (Bruker, 2009), SHELXT (Sheldrick, 2015a), SHELXL97 and SHELXL2018 (Sheldrick, 2015b), ORTEP-3 for Windows (Farrugia, 2012), Mercury (Macrae et al., 2020) and PLATON (Spek, 2020).

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full crystallographic data

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Crystal data

C<sub>20</sub>H<sub>15</sub>ClN<sub>2</sub>O  

*F*(000) = 1392  

*D*<sub>a</sub> = 1.324 Mg m<sup>-3</sup>  

Monoclinic, *C*<sub>2</sub>/c  

Mo *K*<sub>a</sub> radiation, *λ* = 0.71073 Å  

Cell parameters from 2246 reflections  

θ = 2.9–23.5°  

µ = 0.24 mm<sup>-1</sup>  

*T* = 293 K  

Block, colourless  

0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEXII CCD diffractometer  

42189 measured reflections  

2949 independent reflections  

2353 reflections with *I* > 2σ(*I*)  

*R*<sub>int</sub> = 0.056  

θ<sub>max</sub> = 25.5°, θ<sub>min</sub> = 3.2°  

*h* = −36→36  

*k* = −10→10  

*l* = −16→16

Refinement

Refinement on *F*<sub>2</sub>  

Least-squares matrix: full  

*R*<sub>1</sub> = 0.051  

*S* = 1.12  

Hydrogen site location: inferred from neighbouring sites  

H-atom parameters constrained  

\[w = 1/[σ^2(F_c^2) + (0.0578P)^2 + 3.7997P]\]  

where *P* = (*F*<sub>c</sub>² + 2*F*<sub>c</sub>*<sub>o</sub>²) / 3  

(Δ/σ)max < 0.001  

Δρ<sub>max</sub> = 0.39 e Å<sup>-3</sup>  

Δρ<sub>min</sub> = −0.44 e Å<sup>-3</sup>  

Extinction correction: SHELXL2018 (Sheldrick, 2015b),  

Fc = k*Fc*[1+0.001xFe²]/sin(2θ)]<sup>1/4</sup>  

Extinction coefficient: 0.0169 (15)

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.
Refinement. The hydrogen atoms were included in their geometrically calculated positions and refined isotropically with C—H = 0.93 or 0.97 Å and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\AA^2$)**

|       | x       | y       | z       | $U_{\text{iso}}$/$U_{\text{eq}}$ |
|-------|---------|---------|---------|----------------------------------|
| C1    | 0.30506 (10) | 0.5737 (4) | 0.3310 (2) | 0.0788 (9) |
| H1    | 0.3008     | 0.6269   | 0.2702   | 0.095*    |
| C2    | 0.26559 (11) | 0.5226 (5) | 0.3465 (3) | 0.0966 (12) |
| H2    | 0.2345     | 0.5414   | 0.2953   | 0.116*    |
| C3    | 0.27141 (10) | 0.4449 (4) | 0.4359 (3) | 0.0853 (9) |
| H3    | 0.2445     | 0.4113   | 0.4450   | 0.102*    |
| C4    | 0.31708 (10) | 0.4167 (3) | 0.5118 (2) | 0.0706 (7) |
| H4    | 0.3212     | 0.3647   | 0.5729   | 0.085*    |
| C5    | 0.35712 (9) | 0.4656 (3) | 0.49759 (19) | 0.0580 (6) |
| H5    | 0.3881     | 0.4453   | 0.5487   | 0.070*    |
| C6    | 0.35095 (8) | 0.5440 (3) | 0.40771 (17) | 0.0531 (6) |
| C7    | 0.43290 (9) | 0.6267 (3) | 0.30115 (16) | 0.0558 (6) |
| H7    | 0.4422     | 0.6301   | 0.2461   | 0.067*    |
| C8    | 0.46319 (8) | 0.6698 (3) | 0.40535 (15) | 0.0466 (5) |
| C9    | 0.43539 (8) | 0.6472 (2) | 0.46043 (15) | 0.0447 (5) |
| C10   | 0.45229 (8) | 0.6841 (3) | 0.57428 (15) | 0.0490 (5) |
| H10A  | 0.4664     | 0.5931   | 0.6165   | 0.059*    |
| H10B  | 0.4252     | 0.7178   | 0.5882   | 0.059*    |
| C11   | 0.49020 (8) | 0.8128 (3) | 0.60228 (17) | 0.0536 (6) |
| H11A  | 0.4739     | 0.9090   | 0.5720   | 0.064*    |
| H11B  | 0.5055     | 0.8254   | 0.6780   | 0.064*    |
| C12   | 0.52910 (8) | 0.7832 (3) | 0.56429 (16) | 0.0460 (5) |
| C13   | 0.51238 (8) | 0.7266 (3) | 0.45363 (16) | 0.0480 (5) |
| C14   | 0.57663 (8) | 0.8010 (3) | 0.62150 (17) | 0.0503 (5) |
| H14   | 0.5962     | 0.7770   | 0.5876   | 0.060*    |
| C15   | 0.60225 (8) | 0.8534 (3) | 0.73111 (17) | 0.0483 (5) |
| C16   | 0.58651 (9) | 0.9775 (3) | 0.77156 (18) | 0.0545 (6) |
| H16   | 0.5589     | 1.0315   | 0.7278   | 0.065*    |
| C17   | 0.61102 (9) | 1.0221 (3) | 0.87534 (19) | 0.0599 (6) |
| H17   | 0.6002     | 1.1056   | 0.9011   | 0.072*    |
| C18   | 0.65138 (9) | 0.9423 (3) | 0.93968 (19) | 0.0617 (7) |
| C19   | 0.66861 (9) | 0.8207 (3) | 0.9027 (2) | 0.0666 (7) |
| H19   | 0.6962     | 0.7676   | 0.9473   | 0.080*    |
| C20   | 0.64429 (8) | 0.7783 (3) | 0.7983 (2) | 0.0595 (6) |
| H20   | 0.6563     | 0.6978   | 0.7725   | 0.071*    |
| N1    | 0.39190 (7) | 0.5928 (2) | 0.39106 (13) | 0.0502 (5) |
| N2    | 0.39011 (8) | 0.5812 (2) | 0.29111 (14) | 0.0588 (5) |
| O1    | 0.53879 (6) | 0.7264 (2) | 0.40725 (12) | 0.0669 (5) |
| C11   | 0.68147 (4) | 0.99499 (12) | 1.07100 (6) | 0.1050 (4) |
### Atomic displacement parameters (Å²)

| Atom | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|------|----------|----------|----------|----------|----------|----------|
| C1   | 0.0585 (16) | 0.120 (3) | 0.0481 (14) | 0.0063 (16) | 0.0129 (12) | −0.0020 (15) |
| C2   | 0.0489 (15) | 0.156 (3) | 0.0687 (19) | −0.0017 (18) | 0.0097 (14) | −0.014 (2) |
| C3   | 0.0570 (16) | 0.119 (3) | 0.082 (2) | −0.0160 (17) | 0.0322 (15) | −0.0208 (19) |
| C4   | 0.0634 (16) | 0.0813 (19) | 0.0700 (17) | −0.0088 (14) | 0.0310 (14) | −0.0017 (14) |
| C5   | 0.0515 (13) | 0.0658 (15) | 0.0528 (13) | −0.0032 (11) | 0.0185 (11) | −0.0002 (11) |
| C6   | 0.0450 (12) | 0.0638 (14) | 0.0472 (12) | −0.0030 (10) | 0.0163 (10) | −0.0126 (11) |
| C7   | 0.0719 (16) | 0.0620 (14) | 0.0346 (11) | −0.0053 (12) | 0.0235 (11) | −0.0014 (10) |
| C8   | 0.0588 (12) | 0.0498 (12) | 0.0326 (10) | −0.0014 (10) | 0.0205 (9) | −0.0066 (9) |
| C9   | 0.0512 (12) | 0.0463 (12) | 0.0342 (10) | 0.0015 (9) | 0.0159 (9) | −0.0066 (8) |
| C10  | 0.0503 (12) | 0.0643 (14) | 0.0354 (10) | −0.0041 (10) | 0.0208 (9) | −0.0065 (10) |
| C11  | 0.0565 (13) | 0.0652 (14) | 0.0418 (11) | −0.0061 (11) | 0.0234 (10) | −0.0131 (10) |
| C12  | 0.0542 (12) | 0.0478 (12) | 0.0389 (11) | −0.0037 (10) | 0.0225 (9) | −0.0017 (9) |
| C13  | 0.0612 (13) | 0.0496 (12) | 0.0380 (10) | −0.0013 (10) | 0.0256 (10) | 0.0011 (9) |
| C14  | 0.0583 (13) | 0.0526 (13) | 0.0458 (12) | −0.0079 (10) | 0.0278 (10) | −0.0038 (10) |
| C15  | 0.0494 (12) | 0.0484 (12) | 0.0476 (12) | −0.0080 (10) | 0.0211 (10) | −0.0035 (9) |
| C16  | 0.0570 (13) | 0.0497 (13) | 0.0512 (13) | −0.0031 (10) | 0.0175 (11) | −0.0019 (10) |
| C17  | 0.0673 (15) | 0.0550 (14) | 0.0565 (14) | −0.0070 (12) | 0.0253 (12) | −0.0130 (11) |
| C18  | 0.0647 (15) | 0.0654 (16) | 0.0472 (13) | −0.0158 (12) | 0.0162 (12) | −0.0066 (11) |
| C19  | 0.0528 (13) | 0.0643 (16) | 0.0637 (16) | −0.0029 (12) | 0.0064 (12) | −0.0019 (13) |
| C20  | 0.0498 (13) | 0.0578 (14) | 0.0671 (15) | −0.0046 (11) | 0.0211 (12) | −0.0139 (12) |
| N1   | 0.0526 (10) | 0.0598 (12) | 0.0343 (9) | −0.0020 (9) | 0.0146 (8) | −0.0049 (8) |
| N2   | 0.0689 (13) | 0.0686 (13) | 0.0332 (9) | −0.0044 (10) | 0.0163 (9) | −0.0038 (9) |
| O1   | 0.0719 (11) | 0.0929 (14) | 0.0488 (9) | −0.0152 (10) | 0.0382 (9) | −0.0104 (9) |
| C11  | 0.1194 (8) | 0.1189 (8) | 0.0501 (4) | −0.0154 (6) | 0.0101 (4) | −0.0184 (4) |

### Geometric parameters (Å, °)

| Bond | Length (Å) | Angle (°) |
|------|------------|-----------|
| C1—C6 | 1.380 (3) | C10—H10B | 0.9700 |
| C1—C2 | 1.383 (4) | C11—C12 | 1.514 (3) |
| C1—H1 | 0.9300 | C11—H11A | 0.9700 |
| C2—C3 | 1.367 (5) | C11—H11B | 0.9700 |
| C2—H2 | 0.9300 | C12—C14 | 1.335 (3) |
| C3—C4 | 1.370 (4) | C12—C13 | 1.498 (3) |
| C3—H3 | 0.9300 | C13—O1 | 1.232 (2) |
| C4—C5 | 1.384 (3) | C14—C15 | 1.472 (3) |
| C4—H4 | 0.9300 | C14—H14 | 0.9300 |
| C5—C6 | 1.375 (3) | C15—C20 | 1.389 (3) |
| C5—H5 | 0.9300 | C15—C16 | 1.393 (3) |
| C6—N1 | 1.428 (3) | C16—C17 | 1.382 (3) |
| C7—N2 | 1.312 (3) | C16—H16 | 0.9300 |
| C7—C8 | 1.410 (3) | C17—C18 | 1.366 (4) |
| C7—H7 | 0.9300 | C17—H17 | 0.9300 |
| C8—C9 | 1.382 (3) | C18—C19 | 1.373 (4) |
| C8—C13 | 1.445 (3) | C18—C11 | 1.737 (2) |
| C9—N1 | 1.354 (3) | C19—C20 | 1.384 (3) |
C9—C10 1.492 (3)  C10—C19—H19 0.9300
C10—C11 1.532 (3)  C20—H20 0.9300
C10—H10A 0.9700  N1—N2 1.385 (2)
C6—C1—C2 118.6 (3)  C10—C11—H11A 108.8
C6—C1—H1 120.7  C12—C11—H11B 108.8
C2—C1—H1 120.7  C10—C11—H11B 108.8
C3—C2—C1 121.3 (3)  H11A—C11—H11B 107.7
C3—C2—H2 119.4  C14—C12—C13 117.88 (19)
C1—C2—H2 119.4  C14—C12—C11 125.50 (19)
C2—C3—C4 119.7 (3)  C13—C12—C11 116.62 (18)
C2—C3—H3 120.1  O1—C13—C8 122.14 (19)
C4—C3—H3 120.1  O1—C13—C12 122.5 (2)
C3—C4—C5 120.0 (3)  C8—C13—C12 115.31 (18)
C3—C4—H4 120.0  C12—C14—C15 128.6 (2)
C5—C4—H4 120.0  C12—C14—H14 115.7
C6—C5—C4 119.8 (2)  C15—C14—H14 115.7
C6—C5—H5 120.1  C20—C15—C16 117.5 (2)
C4—C5—H5 120.1  C20—C15—C14 119.6 (2)
C5—C6—C1 120.5 (2)  C16—C15—C14 122.9 (2)
C5—C6—N1 120.5 (2)  C17—C16—C15 121.3 (2)
C1—C6—N1 119.0 (2)  C17—C16—H16 119.3
N2—C7—C8 112.04 (19)  C15—C16—H16 119.3
N2—C7—H7 124.0  C18—C17—C16 119.3 (2)
C8—C7—H7 124.0  C18—C17—H17 120.3
C9—C8—C7 104.84 (19)  C16—C17—H17 120.3
C9—C8—C13 123.08 (18)  C17—C18—C19 121.3 (2)
C7—C8—C13 132.08 (19)  C17—C18—Cl1 119.5 (2)
N1—C9—C8 106.97 (18)  C19—C18—Cl1 119.2 (2)
N1—C9—C10 129.34 (19)  C18—C19—C20 119.0 (2)
C8—C9—C10 123.66 (19)  C18—C19—H19 120.5
C9—C10—C11 108.14 (18)  C20—C19—H19 120.5
C9—C10—H10A 110.1  C19—C20—C15 121.4 (2)
C11—C10—H10A 110.1  C19—C20—H20 119.3
C9—C10—H10B 110.1  C15—C20—H20 119.3
C11—C10—H10B 110.1  C9—N1—C6 111.14 (18)
H10A—C10—H10B 108.4  C9—N1—C6 129.95 (17)
C12—C11—C10 113.84 (19)  N2—N1—C6 118.87 (17)
C12—C11—H11A 108.8  C7—N2—N1 105.00 (17)
C6—C1—C2—C3 0.3 (5)  C11—C12—C13—C8 −15.1 (3)
C1—C2—C3—C4 0.0 (6)  C13—C12—C14—C15 −179.6 (2)
C2—C3—C4—C5 −0.6 (5)  C11—C12—C14—C15 −0.8 (4)
C3—C4—C5—C6 0.8 (4)  C12—C14—C15—C20 137.4 (3)
C4—C5—C6—C1 −0.4 (4)  C12—C14—C15—C16 −43.2 (4)
C4—C5—C6—N1 −178.9 (2)  C20—C15—C16—C17 −1.6 (3)
C2—C1—C6—C5 −0.1 (4)  C14—C15—C16—C17 179.0 (2)
C2—C1—C6—N1 178.3 (3)  C15—C16—C17—C18 −0.3 (4)
### Hydrogen-bond geometry (Å, °)

| D—H···A       | D—H | H···A | D···A     | D—H···A |
|---------------|-----|-------|-----------|---------|
| C14—H14···O1  | 0.93| 2.43  | 2.804 (3) | 104     |
| C5—H5···O1i   | 0.93| 2.53  | 3.320 (3) | 143     |
| C7—H7···O1ii  | 0.93| 2.59  | 3.493 (3) | 163     |
| C17—H17···O1iii| 0.93| 2.40  | 3.260 (3) | 154     |
| C2—H2···Cl1iv | 0.93| 2.90  | 3.633 (3) | 137     |

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