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Crystal structure and Hirshfeld surface analysis of a new benzimidazole compound, 3-{1-[(2-hydroxyphenyl)methyl]-1*H*-1,3-benzodiazol-2-yl}phenol

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Keywords: benzimidazole; single crystal; X-ray diffraction; hydrogen bonding; intermolecular interactions; Hirshfeld surface analysis.

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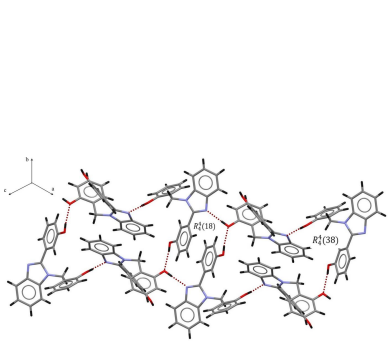
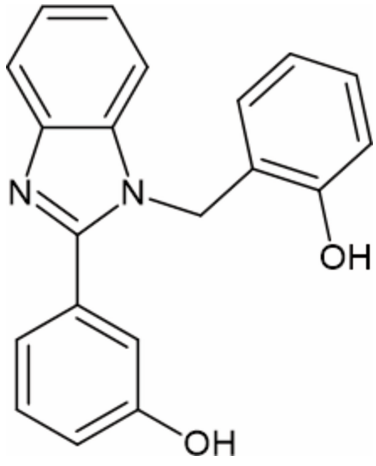
The title compound, $C_{20}H_{16}N_2O_2$, is composed of two monosubstituted benzene rings and one benzimidazole unit. The benzimidazole moiety subtends dihedral angles of 46.16 (7) and 77.45 (8)° with the benzene rings, which themselves form a dihedral angle of 54.34 (9)°. The crystal structure features O—H···N and O—H···O hydrogen-bonding interactions, which together lead to the formation of two-dimensional hydrogen-bonded layers parallel to the (101) plane. In addition, π–π interactions also contribute to the crystal cohesion. Hirshfeld surface analysis indicates that the most significant contacts in the crystal packing are: H···H (47.5%), O···H/H···O (12.4%), N···H/H···N (6.1%), C···H/H···C (27.6%) and C···C (4.6%).

1. Chemical context

The benzimidazole unit comprises a phenyl ring fused to an imidazole ring. The first benzimidazole compound was prepared by Hoebrecker (1872). Benzimidazole is an important structural core in medicinal chemistry and this class of compounds displays a broad range of biological activities such as antimicrobial, antiviral, anticancer, anti-inflammatory, gastroprotective and analgesic (Spasov *et al.*, 1999; Sevak *et al.*, 2002; Demirayak *et al.*, 2005). The use of benzimidazole derivatives with common drugs employed in the treatment of giardiasis has been reviewed (Harris *et al.*, 2001). The coordination behavior of benzimidazole derivatives towards transition-metal ions was explored in order to increase their biological activity (Téllez *et al.*, 2007). The present work describes the synthesis, structural characterization and Hirshfeld analysis of a new benzimidazole compound, 3-{1-[(2-hydroxyphenyl)methyl]-1*H*-1,3-benzodiazol-2-yl}phenol.





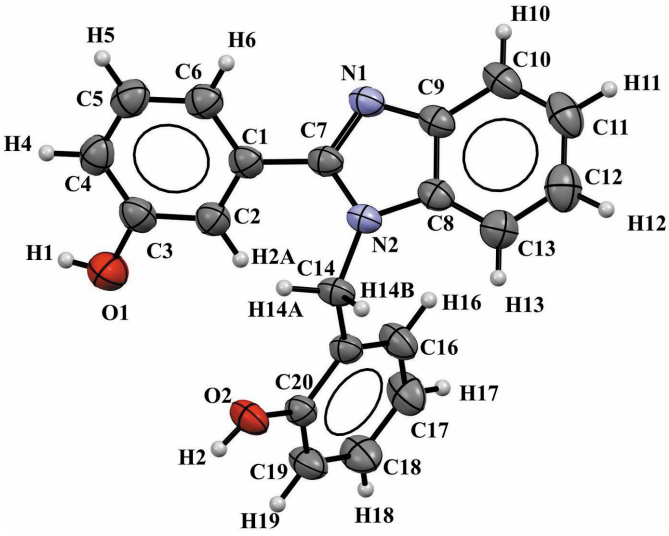


Figure 1
ORTEP view of the title compound with displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

The title compound is composed of two monosubstituted benzene rings and one benzimidazole unit (Fig. 1). The benzimidazole moiety subtends dihedral angles of 46.16 (7) and 77.45 (8)° with the benzene rings, which themselves form a dihedral angle of 54.34 (9)°. These angles are in agreement with those observed in similar structures (Quezada-Miriel *et al.*, 2012; Shu-Ping Yang *et al.*, 2007).

3. Supramolecular features

The crystal packing of the title compound reveals intermolecular hydrogen bonding, specifically O—H···O interactions involving benzene rings and O—H···N interaction between the benzimidazole moieties and benzene rings (Table 1). The molecules are self-assembled by intermolecular hydrogen bonds between the hydroxyl groups and the N1 atoms of the benzimidazole moieties, forming hydrogen-bonded ribbons with a *C*(8) graph-set motif (Etter *et al.*, 1990; Bernstein *et al.*, 1995) parallel to the (111) plane. The combination of the O—H···O and O—H···N hydrogen bonds leads to rings with R_4^4 (18) and R_4^4(38) graph-set motifs (Fig. 2). Further cohesion of the crystal packing is provided by π–π stacking interactions between C1–C6 benzene rings with centroid–centroid distances of 3.5957 (11) Å.

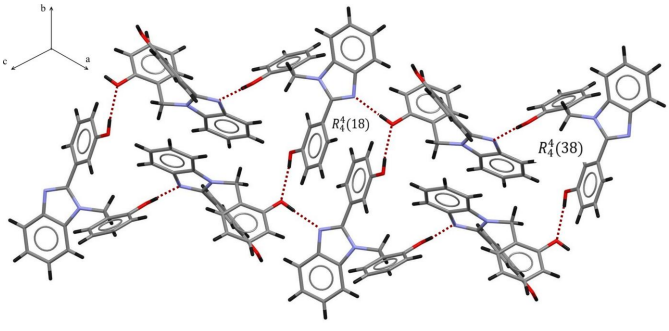


Figure 2
The R_4^4 (18) and R_4^4(38) graph-set motifs parallel to the *ab* plane generated by the combination of O—H···O and O—H···N hydrogen bonds.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	2.04	2.861 (2)	173
O2—H2···N1^{ii}	0.82	1.89	2.7124 (19)	178
C16—H16···N2	0.93	2.55	2.878 (2)	101

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

4. Hirshfeld surface analysis

Hirshfeld surface analysis was undertaken in order to better understand the intermolecular interactions within the crystal structure using graphical tools (Spackman & Jayatilaka, 2009; Spackman *et al.*, 2021). Hirshfeld surface analysis provides a three-dimensional picture of the intermolecular interactions. These interactions can be summarized by using fingerprint plots. The Hirshfeld surface of the title compound mapped over d_{norm} is shown in Fig. 3. The red spots on the surface indicate the presence of atoms in very close proximity to the outside of the surface, the white means that the atoms are in medium proximity while the blue areas are completely devoid of close contacts. The combination of the 3D Hirshfeld surface and the 2D fingerprint plots (Fig. 4), shows that intermolecular H···H contacts make the main contribution, corresponding to 47.5% of the total Hirshfeld surface (McKinnon *et al.*, 2007) and that there are short intermolecular H···H contacts where $d_e = d_i = 1$ Å. In the fingerprint plot delineated into C···H/

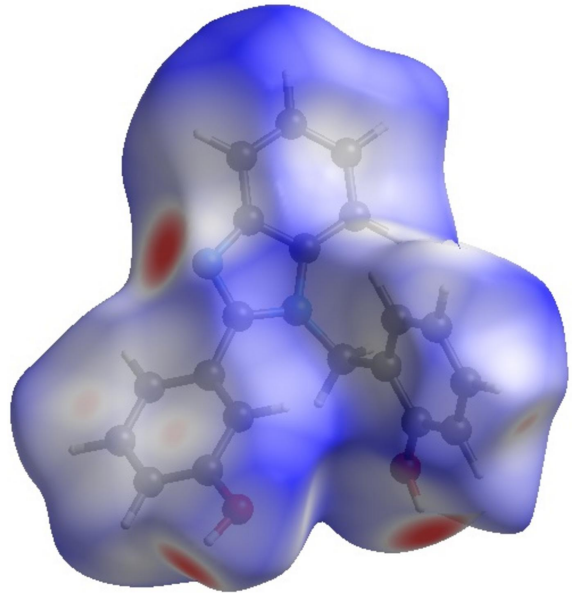


Figure 3
Hirshfeld surface of the title compound mapped with d_{norm}.

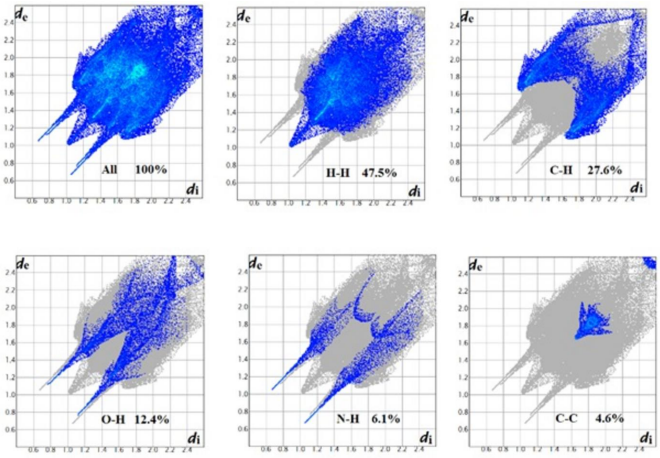


Figure 4
Two-dimensional fingerprints plots of the title compound, showing H···H, C···H/H···C, O···H/H···O, N···H/H···N and C···C contacts.

H···C contacts (27.6% of the total Hirshfeld surface) there are two short spikes. The red spots on the d_{norm} surface in Fig. 3 are due to the H_O···O contacts corresponding to O—H···O and O—H···N hydrogen bonds. The O···H and N···H contacts represent 12.4% and 6.1% of the total Hirshfeld surface, respectively, Fig. 5. These contacts are manifested as sharp spikes at $d_e + d_i$ = 1.8 Å for N···H and 1.9 Å for O···H. Finally, packing cohesion in this structure is also provided by C···N and C···C interactions, which correspond to π–π stacking interactions.

5. Synthesis and crystallization

All chemicals were commercially available, purchased from Sigma-Aldrich, and used as received without purification. 3-Hydroxybenzaldehyde (0.244 g, 2 mmol) and salicylaldehyde (0.244 g, 2 mmol) were added to an ethanolic solution of *o*-phenylenediamine (0.216 g, 2 mmol). The reaction mixture was stirred for 4 h under reflux at 348 K. The resulting brown solution was cooled in an ice bath. The obtained filtrate was left to evaporate slowly at room temperature, giving after two weeks colorless crystals suitable for single-crystal x-ray diffraction analysis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were located in difference electron-density maps and were treated as riding on their parent atoms with C—H = 0.93 Å, O—H = 0.84 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

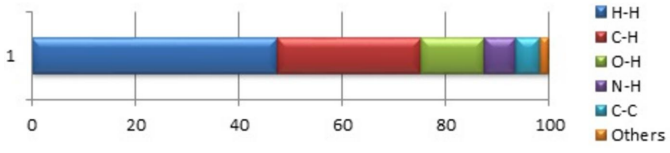


Figure 5
Relative contributions of various interactions to the Hirshfeld surface area of the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{16}N_2O_2$
M_r	316.35
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	10.6474 (3), 13.2429 (3), 11.4176 (3)
β (°)	99.067 (1)
V (Å^3)	1589.79 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.1 × 0.1 × 0.08
Data collection	
Diffractometer	Nonius KappaCCD
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33506, 4650, 2866
R_{int}	0.056
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.059, 0.190, 1.06
No. of reflections	4643
No. of parameters	217
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.50, −0.30

Computer programs: *COLLECT* (Nonius, 1999), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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Zakaria Bouhidel, Kaouther Sahli and Aouatef Cherouana

Computing details

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Crystal data

$C_{20}H_{16}N_2O_2$
M_r = 316.35
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.6474 (3) Å
b = 13.2429 (3) Å
c = 11.4176 (3) Å
β = 99.067 (1)°
V = 1589.79 (7) Å^3
Z = 4
F(000) = 664

Least Squares Treatment of 25 SET4 setting angles.
D_x = 1.322 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 33506 reflections
θ = 2.4–30.1°
μ = 0.09 mm^{-1}
T = 100 K
Prism, colourless
0.1 × 0.1 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
33506 measured reflections
4650 independent reflections

2866 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 30.1°, θ_{min} = 2.4°
h = −15→14
k = −17→18
l = −15→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.190
S = 1.06
4643 reflections
217 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
W = 1/[Σ^2(FO^2) + (0.1027P)^2 + 0.1399P] WHERE P = (FO^2 + 2FC^2)/3
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.71485 (14)	0.50588 (12)	0.85134 (15)	0.0674 (6)
O2	0.86823 (12)	0.19463 (10)	0.75574 (10)	0.0484 (4)
N1	0.50090 (14)	0.18753 (11)	1.12414 (12)	0.0415 (4)
N2	0.64015 (13)	0.13212 (10)	1.01162 (12)	0.0365 (4)
C1	0.54208 (16)	0.30396 (13)	0.96699 (14)	0.0393 (5)
C2	0.64184 (18)	0.36170 (13)	0.93853 (15)	0.0434 (5)
C3	0.61480 (19)	0.45154 (14)	0.87656 (16)	0.0470 (6)
C4	0.49058 (19)	0.48277 (14)	0.84368 (16)	0.0496 (6)
C5	0.3922 (2)	0.42579 (16)	0.87286 (17)	0.0524 (6)
C6	0.41675 (19)	0.33701 (15)	0.93432 (16)	0.0475 (6)
C7	0.56219 (15)	0.20898 (13)	1.03474 (14)	0.0376 (5)
C8	0.62905 (16)	0.05631 (12)	1.09273 (15)	0.0386 (5)
C9	0.54146 (16)	0.09200 (13)	1.16216 (15)	0.0405 (5)
C10	0.50993 (19)	0.03349 (15)	1.25517 (17)	0.0504 (6)
C11	0.5675 (2)	−0.05921 (16)	1.27507 (19)	0.0584 (7)
C12	0.6536 (2)	−0.09453 (14)	1.20405 (19)	0.0573 (7)
C13	0.68637 (19)	−0.03791 (14)	1.11183 (17)	0.0485 (6)
C14	0.71836 (15)	0.12707 (14)	0.91676 (14)	0.0389 (5)
C15	0.85421 (16)	0.16113 (12)	0.95674 (14)	0.0353 (5)
C16	0.91028 (19)	0.16091 (16)	1.07445 (16)	0.0500 (6)
C17	1.0337 (2)	0.19263 (17)	1.10898 (18)	0.0565 (7)
C18	1.10283 (19)	0.22691 (18)	1.02536 (18)	0.0561 (7)
C19	1.04917 (17)	0.22814 (16)	0.90709 (17)	0.0505 (6)
C20	0.92539 (16)	0.19490 (12)	0.87220 (14)	0.0364 (5)
H1	0.69016	0.56161	0.82622	0.1010*
H2	0.90990	0.22934	0.71643	0.0730*
H2A	0.72555	0.34062	0.96058	0.0520*
H4	0.47340	0.54263	0.80161	0.0590*
H5	0.30871	0.44742	0.85090	0.0630*
H6	0.34993	0.29882	0.95425	0.0570*
H10	0.45194	0.05650	1.30205	0.0600*
H11	0.54868	−0.09918	1.33701	0.0700*
H12	0.68991	−0.15799	1.21930	0.0690*
H13	0.74390	−0.06162	1.06486	0.0580*
H14A	0.68017	0.16920	0.85120	0.0470*
H14B	0.71891	0.05813	0.88814	0.0470*
H16	0.86349	0.13880	1.13176	0.0600*
H17	1.06999	0.19081	1.18856	0.0680*
H18	1.18584	0.24933	1.04831	0.0670*
H19	1.09626	0.25138	0.85055	0.0610*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0589 (9)	0.0611 (9)	0.0872 (12)	0.0017 (7)	0.0269 (8)	0.0158 (8)

O2	0.0457 (7)	0.0684 (8)	0.0323 (6)	−0.0122 (6)	0.0096 (5)	0.0031 (5)
N1	0.0386 (8)	0.0533 (8)	0.0348 (7)	0.0000 (6)	0.0125 (6)	−0.0014 (6)
N2	0.0342 (7)	0.0432 (7)	0.0342 (7)	−0.0025 (6)	0.0118 (6)	−0.0014 (5)
C1	0.0426 (9)	0.0459 (9)	0.0300 (8)	0.0020 (7)	0.0080 (7)	−0.0044 (6)
C2	0.0446 (10)	0.0482 (9)	0.0383 (9)	0.0035 (8)	0.0092 (8)	−0.0003 (7)
C3	0.0536 (11)	0.0493 (10)	0.0407 (10)	−0.0016 (8)	0.0157 (8)	−0.0028 (7)
C4	0.0579 (12)	0.0499 (10)	0.0395 (10)	0.0095 (9)	0.0034 (8)	0.0003 (8)
C5	0.0495 (11)	0.0612 (11)	0.0446 (10)	0.0083 (9)	0.0012 (8)	−0.0028 (9)
C6	0.0458 (10)	0.0550 (10)	0.0418 (10)	0.0037 (8)	0.0072 (8)	−0.0037 (8)
C7	0.0346 (8)	0.0475 (9)	0.0312 (8)	−0.0019 (7)	0.0068 (6)	−0.0039 (6)
C8	0.0349 (8)	0.0438 (8)	0.0370 (9)	−0.0085 (7)	0.0058 (7)	−0.0033 (7)
C9	0.0365 (9)	0.0489 (9)	0.0371 (9)	−0.0074 (7)	0.0089 (7)	−0.0024 (7)
C10	0.0487 (11)	0.0623 (11)	0.0426 (10)	−0.0139 (9)	0.0146 (8)	0.0028 (8)
C11	0.0643 (13)	0.0582 (12)	0.0519 (12)	−0.0225 (10)	0.0063 (10)	0.0102 (9)
C12	0.0674 (14)	0.0410 (9)	0.0600 (12)	−0.0101 (9)	−0.0006 (10)	0.0029 (9)
C13	0.0506 (11)	0.0445 (9)	0.0505 (11)	−0.0031 (8)	0.0081 (9)	−0.0044 (8)
C14	0.0360 (9)	0.0501 (9)	0.0325 (8)	−0.0039 (7)	0.0117 (7)	−0.0054 (7)
C15	0.0343 (8)	0.0411 (8)	0.0317 (8)	0.0004 (6)	0.0085 (6)	−0.0022 (6)
C16	0.0484 (11)	0.0690 (12)	0.0331 (9)	−0.0117 (9)	0.0076 (8)	0.0055 (8)
C17	0.0517 (12)	0.0776 (14)	0.0362 (10)	−0.0147 (10)	−0.0051 (8)	0.0049 (9)
C18	0.0373 (10)	0.0784 (13)	0.0500 (11)	−0.0128 (9)	−0.0007 (8)	0.0048 (10)
C19	0.0382 (10)	0.0718 (12)	0.0432 (10)	−0.0084 (9)	0.0120 (8)	0.0076 (9)
C20	0.0370 (9)	0.0427 (8)	0.0304 (8)	0.0018 (7)	0.0077 (7)	−0.0008 (6)

Geometric parameters (Å, º)

O1—C3	1.354 (3)	C14—C15	1.515 (2)
O2—C20	1.372 (2)	C15—C20	1.392 (2)
N1—C7	1.326 (2)	C15—C16	1.382 (2)
N1—C9	1.384 (2)	C16—C17	1.377 (3)
O1—H1	0.8200	C17—C18	1.372 (3)
N2—C7	1.365 (2)	C18—C19	1.381 (3)
N2—C14	1.468 (2)	C19—C20	1.387 (3)
O2—H2	0.8200	C2—H2A	0.9300
N2—C8	1.384 (2)	C4—H4	0.9300
C1—C6	1.398 (3)	C5—H5	0.9300
C1—C2	1.388 (3)	C6—H6	0.9300
C1—C7	1.475 (2)	C10—H10	0.9300
C2—C3	1.391 (3)	C11—H11	0.9300
C3—C4	1.380 (3)	C12—H12	0.9300
C4—C5	1.374 (3)	C13—H13	0.9300
C5—C6	1.373 (3)	C14—H14A	0.9700
C8—C13	1.391 (2)	C14—H14B	0.9700
C8—C9	1.398 (2)	C16—H16	0.9300
C9—C10	1.398 (3)	C17—H17	0.9300
C10—C11	1.375 (3)	C18—H18	0.9300
C11—C12	1.397 (3)	C19—H19	0.9300
C12—C13	1.382 (3)		

C7—N1—C9	105.67 (14)	C17—C18—C19	119.99 (19)
C3—O1—H1	109.00	C18—C19—C20	120.34 (18)
C7—N2—C14	127.55 (14)	C15—C20—C19	119.96 (15)
C8—N2—C14	125.38 (14)	O2—C20—C15	117.67 (15)
C7—N2—C8	107.03 (13)	O2—C20—C19	122.37 (15)
C20—O2—H2	109.00	C1—C2—H2A	120.00
C6—C1—C7	117.43 (16)	C3—C2—H2A	120.00
C2—C1—C6	119.90 (16)	C3—C4—H4	120.00
C2—C1—C7	122.65 (15)	C5—C4—H4	120.00
C1—C2—C3	119.05 (17)	C4—C5—H5	120.00
C2—C3—C4	120.49 (18)	C6—C5—H5	120.00
O1—C3—C2	117.14 (18)	C1—C6—H6	120.00
O1—C3—C4	122.37 (17)	C5—C6—H6	120.00
C3—C4—C5	120.27 (18)	C9—C10—H10	121.00
C4—C5—C6	120.21 (19)	C11—C10—H10	121.00
C1—C6—C5	120.08 (18)	C10—C11—H11	119.00
N1—C7—C1	122.56 (15)	C12—C11—H11	119.00
N1—C7—N2	112.15 (15)	C11—C12—H12	119.00
N2—C7—C1	125.24 (14)	C13—C12—H12	119.00
N2—C8—C13	132.39 (16)	C8—C13—H13	122.00
C9—C8—C13	121.99 (16)	C12—C13—H13	122.00
N2—C8—C9	105.62 (14)	N2—C14—H14A	109.00
C8—C9—C10	120.33 (16)	N2—C14—H14B	109.00
N1—C9—C8	109.52 (15)	C15—C14—H14A	109.00
N1—C9—C10	130.13 (16)	C15—C14—H14B	109.00
C9—C10—C11	117.80 (18)	H14A—C14—H14B	108.00
C10—C11—C12	121.29 (19)	C15—C16—H16	119.00
C11—C12—C13	121.90 (18)	C17—C16—H16	119.00
C8—C13—C12	116.69 (18)	C16—C17—H17	120.00
N2—C14—C15	112.94 (13)	C18—C17—H17	120.00
C16—C15—C20	118.44 (16)	C17—C18—H18	120.00
C14—C15—C16	122.54 (15)	C19—C18—H18	120.00
C14—C15—C20	119.02 (14)	C18—C19—H19	120.00
C15—C16—C17	121.63 (18)	C20—C19—H19	120.00
C16—C17—C18	119.63 (19)		

C9—N1—C7—N2	0.45 (19)	C3—C4—C5—C6	−0.4 (3)
C9—N1—C7—C1	178.12 (15)	C4—C5—C6—C1	−0.3 (3)
C7—N1—C9—C8	−0.12 (19)	N2—C8—C9—N1	−0.25 (19)
C7—N1—C9—C10	178.39 (19)	N2—C8—C9—C10	−178.92 (16)
C8—N2—C7—N1	−0.62 (19)	C13—C8—C9—N1	179.53 (16)
C8—N2—C7—C1	−178.22 (15)	C13—C8—C9—C10	0.9 (3)
C14—N2—C7—N1	177.32 (15)	N2—C8—C13—C12	179.02 (18)
C14—N2—C7—C1	−0.3 (3)	C9—C8—C13—C12	−0.7 (3)
C7—N2—C8—C9	0.51 (18)	N1—C9—C10—C11	−178.49 (18)
C7—N2—C8—C13	−179.25 (19)	C8—C9—C10—C11	−0.1 (3)
C14—N2—C8—C9	−177.49 (15)	C9—C10—C11—C12	−0.7 (3)

C14—N2—C8—C13	2.8 (3)	C10—C11—C12—C13	0.9 (3)
C7—N2—C14—C15	94.94 (19)	C11—C12—C13—C8	−0.2 (3)
C8—N2—C14—C15	−87.5 (2)	N2—C14—C15—C16	22.2 (2)
C6—C1—C2—C3	−0.6 (3)	N2—C14—C15—C20	−157.17 (15)
C7—C1—C2—C3	−178.60 (16)	C14—C15—C16—C17	−179.68 (19)
C2—C1—C6—C5	0.8 (3)	C20—C15—C16—C17	−0.3 (3)
C7—C1—C6—C5	178.91 (17)	C14—C15—C20—O2	−0.6 (2)
C2—C1—C7—N1	134.27 (18)	C14—C15—C20—C19	178.84 (16)
C2—C1—C7—N2	−48.4 (2)	C16—C15—C20—O2	−179.98 (16)
C6—C1—C7—N1	−43.8 (2)	C16—C15—C20—C19	−0.6 (3)
C6—C1—C7—N2	133.60 (18)	C15—C16—C17—C18	1.0 (3)
C1—C2—C3—O1	179.55 (16)	C16—C17—C18—C19	−0.9 (3)
C1—C2—C3—C4	−0.1 (3)	C17—C18—C19—C20	0.0 (3)
O1—C3—C4—C5	−179.00 (18)	C18—C19—C20—O2	−179.92 (19)
C2—C3—C4—C5	0.6 (3)	C18—C19—C20—C15	0.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	2.04	2.861 (2)	173
O2—H2···N1^{ii}	0.82	1.89	2.7124 (19)	178
C16—H16···N2	0.93	2.55	2.878 (2)	101

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