Crystal structure, Hirshfeld and electronic transition analysis of 2-[(1H-benzimidazol-1-yl)-methyl]benzoic acid

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In the title compound, $C_{15}H_{12}N_2O_2$, the benzimidazole ring system is inclined to the benzene ring by 78.04 (10)°. The crystal structure features O—H⋯N and C—H⋯O hydrogen bonding and C—H⋯π and π–π interactions, which were investigated using Hirshfeld surface analysis.
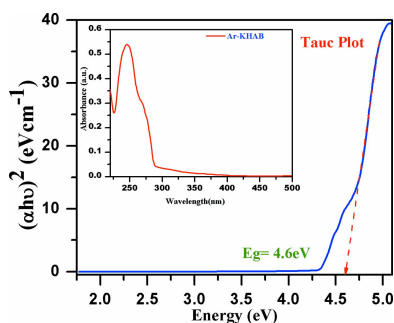
1. Chemical context

Benzimidazole is a naturally ocurring compound, being present in vitamin B_{12} (Crofts *et al.*, 2014) and may also be synthesized from benzoic acid and *o*-phenylenediamine in presence of an excess of acid. Benzimidazole and its derivatives show biological activities such as antibacterial, antifungal (Yadav *et al.*, 2015), antimicrobial (Shruthi *et al.*, 2016), and anticancer (Kalalbandi *et al.*, 2015). Cyanobenzyl compounds are used as intermediates in the synthesis of species that possess significant pharmaceutical properties. Compounds having carboxylic acid as a functional group have shown chelating properties and thus have potential applications in the field of biology. Such groups are also helpful in building metal–organic frameworks that usually form supramolecular networks due to extensive hydrogen bonding and weak interactions. For example, 4-[(1H-benzo[d]imidazol-1-yl)-methyl]benzoic acid has been used to construct coordination polymers with different metal ions (Ahmad *et al.*, 2013). Herein, we report the title compound, 2-[(1H-benzimidazol-1-yl)methyl]benzoic acid, which was synthesized by a condensation reaction of benzimidazole and 2-(bromomethyl)benzonitrile in acetonitrile followed by a hydrolysis process.

2. Structural commentary

The asymmetric unit of the title compound is illustrated in Fig. 1. The molecule is non-planar with a dihedral angle of
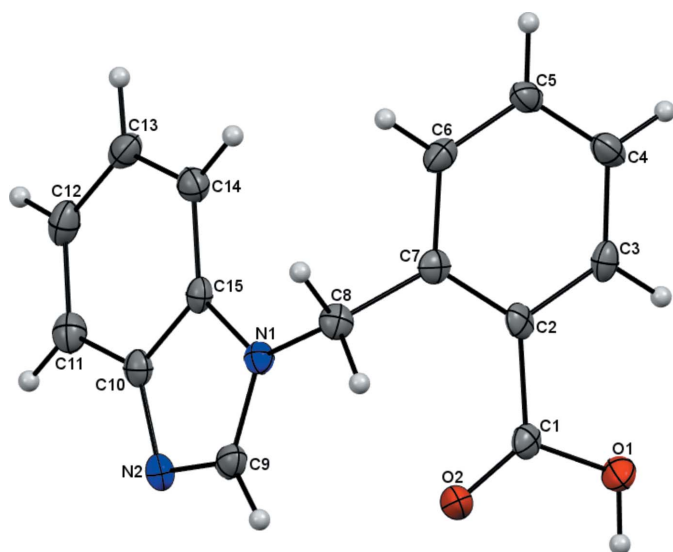
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Figure 1
Asymmetric unit of title compound, with atom labelling and displacement ellipsoids are drawn at the 50% probability level.

78.04 (10) between the benzimidazole ring system and the benzene ring. The N1—C8—C7 angle is 113.31° and the C9—N1—C8—C7 torsion angle is −116.8 (2)°,. The C10—C15 bond length [1.408 (3) Å] is comparable to that in a similar benzimidazole derivative (Faizi *et al.*, 2017). The C—O bond lengths [C1—O1 = 1.319 (3) and C1—O2 = 1.216 (3) Å] are in the expected range (Kamaal *et al.*, 2019).

3. Supramolecular features

In the crystal, the molecules are connected *via* O—H···N and C—H···O hydrogen bonds (Table 1), forming a 1D framework along the *b*-axis direction (Fig. 2). C—H···π and π–π interactions [centroid–centroid distance = 3.6166 (15) Å] between the N1/N2/C9/C10/C15 and C2–C7 rings also occur, leading to the formation of the supramolecular structure (Fig. 3).
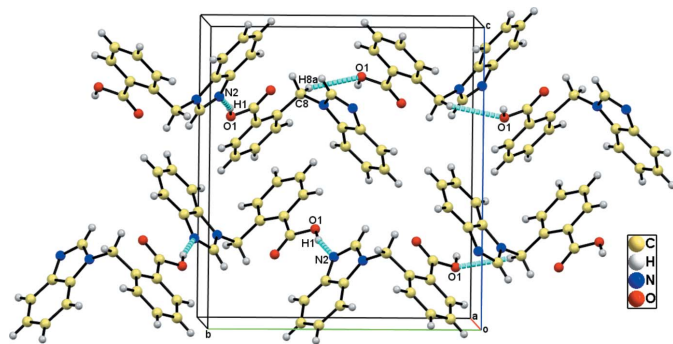
Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N1/N2/C9/C10/C15, C2–C7, C10–C15 and N1/N2/C9–15 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2[i]	0.88 (3)	1.73 (3)	2.592 (3)	164 (4)
C8—H8A···O1[ii]	0.99 (1)	2.62 (1)	3.374 (3)	133 (1)
C4—H4···*Cg*1[iii]	0.95 (1)	2.99 (1)	3.865 (3)	155 (1)
C4—H4···*Cg*3[iii]	0.95 (1)	2.51 (1)	3.408 (3)	157 (1)
C4—H4···*Cg*4[iii]	0.95 (1)	2.51 (1)	3.454 (3)	170 (1)
C5—H5···*Cg*2[iii]	0.95 (1)	2.76 (1)	3.554 (3)	142 (1)

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

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42, November 2020; Groom *et al.*, 2016) found five examples of similar compounds: bis(pentafluorophenyl)-(μ-{1,1′-[1,2-phenylenebis(methylene)]bis(1*H*-benzimidazole)})-digold(I) acetone solvate (WOPLIZ; Zheng *et al.*, 2019), 3,3′-[1,2-phenylenebis(methylene)]bis(1-ethylbenzimidazolium) dibromide (LANHAL; Haque *et al.*, 2012), 2-[(1*H*-benzimidazol-1-yl)methyl]benzonitrile (JONYUJ; Akkoç *et al.*, 2017), 1-[(2-cyanophenyl)methyl]-3-[(2-methylphenyl)methyl]-1*H*-benzimidazol-3-ium (JONZAQ; Akkoç *et al.*, 2017) and 1-(2-cyanobenzyl)-3-methyl-1*H*-3,1-benzimidazol-3-ium bromide (MOCWAE; Ghdhayeb *et al.*, 2014).

5. Hirshfeld surface analysis

A Hirshfeld surface analysis was performed and the two-dimensional fingerprint plots generated (McKinnon *et al.*, 2007; Spackman & Jayatilaka *et al.*, 2009) using Crystal-Explorer17 (Turner *et al.*, 2017). The Hirshfeld surface mapped over d_{norm}, colour-mapped from red (shorter distance than the sum of van der Waals radii) through white to blue

Figure 2
View of the crystal packing along the *a* axis, showing O—H···N and C—H···O hydrogen-bonding interactions forming a one-dimensional chain.
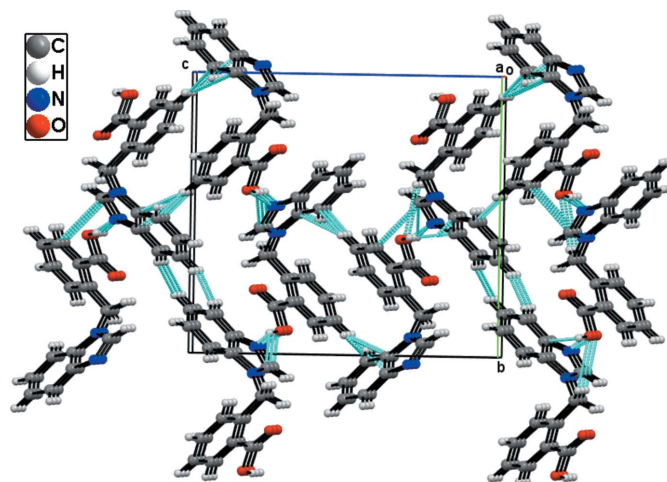

Figure 3
The hydrogen bonding and C—H···π and π–π interactions form zigzag chains, giving a supramolecular structure along the *bc* plane.
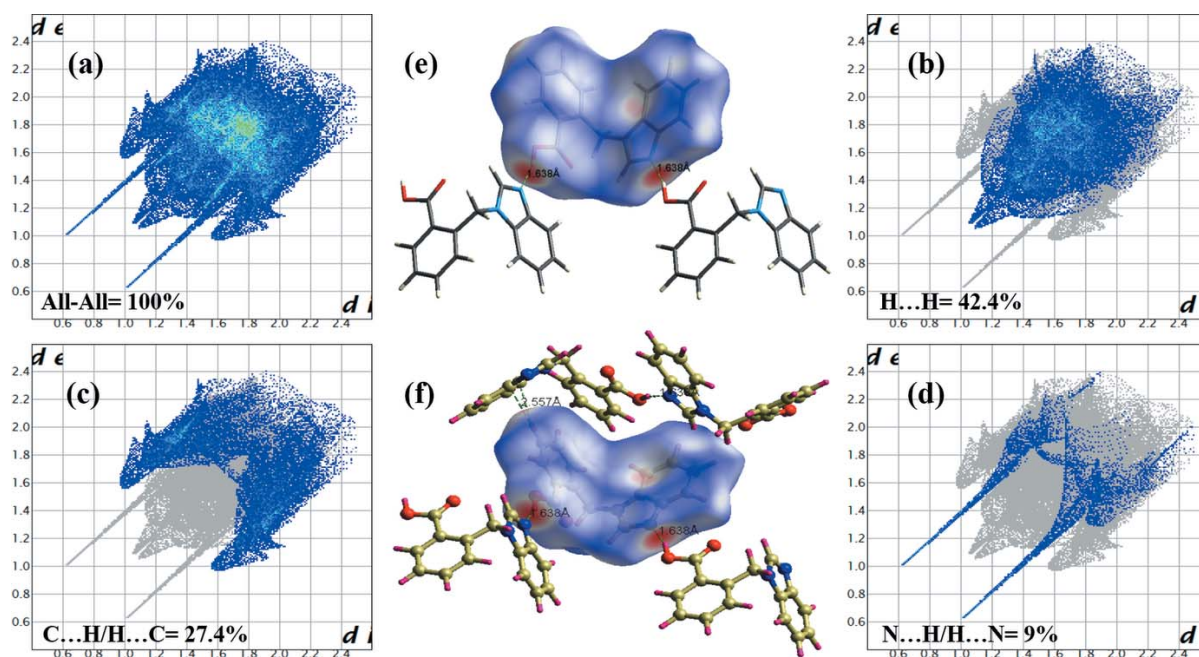
Figure 4
The Hirshfeld surface of the title compound mapped over d_{norm}, in the range −0.722 to 1.183. (*a*) The overall two-dimensional finger plot of the title compound and those delineated into (*b*) H···H (42.4%), (*c*) C···H/ H···C (27.4%) and (*d*) N···H/H···N (9%) interactions, (*e*) significant hydrogen bonding and (*f*) extended supramolecular form.

(longer distance than the sum of the van der Waals radii). The principal weak interactions are clearly visible. The surface coverage corresponding to O—H···N and C—H···O interactions are 9% and 11.8%, respectively. The dark-red spot indicates significant hydrogen bonding.

The two-dimensional finger plots are given in Fig. 4. The principal contributions to the overall surface are from H···H (42.4%, Fig. 4*b*), C···H/H···C (27.4%, Fig. 4*c*) and N···H/ H···N 9% (Fig. 4*d*) interactions. The contributions of interactions such as C···C 4.8% are negligible.

6. Electronic transition analysis

Electro-conducting materials synthesized by conjugated organic compounds show promising electronic properties due to the availability of delocalized electrons, except for semi-conducting materials such as TiO_2, ZnO and other metal oxide nano-materials, which are electro-conducting in themselves (Odziomek *et al.*, 2017). The electronic properties of organic compounds depend on the electronic transition between the highest occupied molecular orbital (HOMO) or valence band and lowest occupied molecular orbital (LUMO) or conduction band. In a simple method, the energy band gap (*Eg*) of organic molecule is determined by a Tauc plot from the absorption spectra (λ_{max} = 245 nm, in this case). The band gap energy, *Eg* = 4.6 eV, of the title compound is very large (Fig. 5). This large band gap arises due to high π-conjugation or polarization in the title molecule system. The title molecule could be useful for developing or enhancing the organic electronic properties of conducting materials such as metal–organic frameworks.

7. Synthesis and crystallization

In an equimolar ratio, benzimidazole (2 g, 16.9 mmol) and dry K_2CO_3 (4.66 g, 33.85 mmol) were mixed in a round-bottom flask in acetonitrile (MeCN, 60 ml) under an inert atmosphere. The mixture was then allowed to stirred for 60 min at 363 K then treated with 2-(bromomethyl) benzonitrile (3.31 g, 16.9 mmol), and the resulting solution refluxed for 24 h. After completion of this step, the solution was allowed to cool to room temperature and the mixture was poured slowly onto
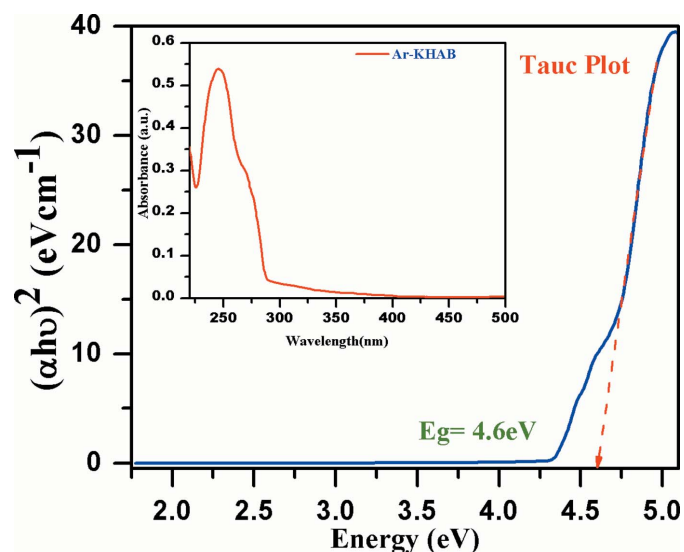

Figure 5
Energy band gap of the title molecule by Tauc plot from absorption spectra.
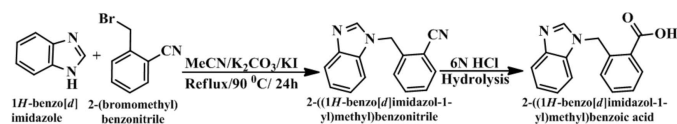
Figure 6
Reaction scheme.

ice–water (100 ml) under constant stirring. A greenish muddy crystalline precipitate was obtained and it was left to stand at 293 K for two days. After two days, a crystalline powder of 2-[(1*H*-benzo[*d*]imidazol-1-yl)methyl]benzonitrile was obtained (Ahmad *et al.*, 2013).

The title compound was synthesized by hydrolysis of 2-[(1*H*-benzo[*d*]imidazol-1-yl)methyl]benzonitrile, 2 g being mixed with 20 equimolar of potassium hydroxide (6.86 g, 8.58 mmol) in water. The solution was refluxed at 373 K for 36 h, the resultant solution was then allowed to cool at room temperature and then poured onto ice–water, and after that acidified using 6 *N* HCl for protonation. The protonated solution was kept for slow evaporation. After two weeks, pale-yellow cubic crystals were obtained in good yield, which were suitable for data collection. The reaction scheme is shown in Fig. 6.

8. Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{12}N_2O_2$
M_r	252.28
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, b, c (Å)	6.5690 (8), 12.7956 (15), 14.1278 (16)
V (Å^3)	1187.5 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	$0.38 \times 0.21 \times 0.14$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	18798, 2095, 1759
R_{int}	0.107
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.091, 1.09
No. of reflections	2095
No. of parameters	176
No. of restraints	1
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.28

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *olex2.solve* (Bourhis *et al.*, 2015), *olex2.refine* (Bourhis *et al.*, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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Crystal structure, Hirshfeld and electronic transition analysis of 2-[(1*H*-benzimidazol-1-yl)methyl]benzoic acid

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Computing details

Data collection: *APEX2* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *olex2.solve* (Bourhis *et al.*, 2015); program(s) used to refine structure: *olex2.refine* (Bourhis *et al.*, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

2-[(1*H*-Benzimidazol-1-yl)methyl]benzoic acid

Crystal data

$C_{15}H_{12}N_2O_2$	$D_x = 1.411$ Mg m^{-3}
$M_r = 252.28$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 1209 reflections
$a = 6.5690$ (8) Å	$\theta = 2.9$–$22.1°$
$b = 12.7956$ (15) Å	$\mu = 0.10$ mm^{-1}
$c = 14.1278$ (16) Å	$T = 100$ K
$V = 1187.5$ (2) Å^3	Block, colourless
$Z = 4$	$0.38 \times 0.21 \times 0.14$ mm
$F(000) = 528.253$	

Data collection

Bruker APEXII CCD diffractometer	2095 independent reflections
	1759 reflections with $I \geq 2u(I)$
Detector resolution: X-ray pixels mm^{-1}	$R_{int} = 0.107$
φ and ω scans	$\theta_{max} = 25.1°$, $\theta_{min} = 3.2°$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$h = -8 \rightarrow 8$
	$k = -17 \rightarrow 17$
	$l = -18 \rightarrow 18$
18798 measured reflections	

Refinement

Refinement on F^2	21 constraints
Least-squares matrix: full	Primary atom site location: iterative
$R[F^2 > 2\sigma(F^2)] = 0.044$	All H-atom parameters refined
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 0.3178P]$
$S = 1.09$	where $P = (F_o^2 + 2F_c^2)/3$
2095 reflections	$(\Delta/\sigma)_{max} = 0.004$
176 parameters	$\Delta\rho_{max} = 0.24$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.28$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2861 (4)	0.82904 (18)	0.71973 (18)	0.0170 (6)
C2	0.4789 (4)	0.81263 (19)	0.66504 (18)	0.0166 (6)
C3	0.5267 (4)	0.88501 (19)	0.59451 (17)	0.0186 (6)
H3	0.4333 (4)	0.93965 (19)	0.58083 (17)	0.0223 (8)*
C4	0.7074 (4)	0.8790 (2)	0.54393 (18)	0.0213 (6)
H4	0.7359 (4)	0.9282 (2)	0.49537 (18)	0.0256 (8)*
C5	0.8447 (4)	0.80132 (19)	0.56462 (18)	0.0204 (7)
H5	0.9705 (4)	0.79769 (19)	0.53166 (18)	0.0245 (8)*
C6	0.7985 (4)	0.7280 (2)	0.63408 (18)	0.0196 (6)
H6	0.8941 (4)	0.6743 (2)	0.64778 (18)	0.0235 (7)*
C7	0.6164 (4)	0.7311 (2)	0.68391 (17)	0.0163 (6)
C8	0.5804 (4)	0.6465 (2)	0.75638 (17)	0.0179 (6)
H8a	0.7114 (4)	0.6115 (2)	0.77035 (17)	0.0215 (7)*
H8b	0.5313 (4)	0.6790 (2)	0.81572 (17)	0.0215 (7)*
C9	0.2503 (4)	0.54778 (19)	0.76721 (18)	0.0197 (6)
H9	0.2023 (4)	0.58470 (19)	0.82111 (18)	0.0236 (7)*
C10	0.2677 (4)	0.43913 (19)	0.65142 (17)	0.0176 (6)
C11	0.2311 (4)	0.3622 (2)	0.58413 (19)	0.0229 (6)
H11	0.1089 (4)	0.3224 (2)	0.58480 (19)	0.0274 (8)*
C12	0.3793 (4)	0.3456 (2)	0.51608 (19)	0.0248 (7)
H12	0.3580 (4)	0.2940 (2)	0.46874 (19)	0.0297 (8)*
C13	0.5601 (4)	0.40366 (19)	0.51595 (18)	0.0223 (7)
H13	0.6590 (4)	0.39013 (19)	0.46844 (18)	0.0267 (8)*
C14	0.5993 (4)	0.4801 (2)	0.58275 (18)	0.0197 (6)
H14	0.7226 (4)	0.5188 (2)	0.58240 (18)	0.0236 (8)*
C15	0.4494 (4)	0.49744 (19)	0.65048 (17)	0.0156 (6)
N1	0.4321 (3)	0.56758 (15)	0.72553 (14)	0.0158 (5)
N2	0.1467 (3)	0.47270 (16)	0.72598 (15)	0.0195 (5)
O1	0.1923 (3)	0.91615 (15)	0.69535 (13)	0.0228 (5)
O2	0.2246 (3)	0.77045 (13)	0.78116 (12)	0.0227 (4)
H1	0.078 (4)	0.924 (3)	0.727 (2)	0.077 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0165 (14)	0.0131 (13)	0.0214 (14)	−0.0029 (12)	−0.0021 (12)	−0.0043 (12)
C2	0.0186 (14)	0.0126 (13)	0.0184 (14)	−0.0064 (11)	−0.0017 (12)	−0.0040 (11)
C3	0.0246 (16)	0.0118 (14)	0.0193 (14)	0.0002 (12)	−0.0039 (12)	−0.0027 (11)
C4	0.0257 (16)	0.0207 (14)	0.0175 (14)	−0.0068 (13)	0.0054 (13)	−0.0014 (12)
C5	0.0217 (15)	0.0172 (14)	0.0223 (16)	−0.0060 (12)	0.0068 (12)	−0.0042 (12)
C6	0.0187 (14)	0.0166 (13)	0.0235 (15)	0.0024 (12)	−0.0007 (12)	−0.0050 (12)
C7	0.0166 (13)	0.0158 (14)	0.0164 (13)	−0.0037 (12)	−0.0020 (11)	−0.0056 (11)
C8	0.0166 (13)	0.0181 (14)	0.0190 (14)	−0.0010 (12)	−0.0033 (12)	−0.0009 (12)
C9	0.0241 (15)	0.0163 (14)	0.0186 (14)	0.0038 (12)	0.0022 (13)	0.0027 (12)
C10	0.0210 (14)	0.0149 (13)	0.0170 (13)	0.0010 (12)	−0.0025 (12)	0.0032 (11)

C11	0.0235 (15)	0.0183 (14)	0.0268 (15)	−0.0006 (13)	−0.0034 (13)	0.0007 (12)
C12	0.0339 (17)	0.0159 (14)	0.0244 (16)	0.0026 (14)	−0.0028 (14)	−0.0030 (13)
C13	0.0295 (17)	0.0185 (15)	0.0188 (14)	0.0077 (12)	0.0031 (13)	0.0007 (12)
C14	0.0201 (15)	0.0178 (14)	0.0212 (14)	−0.0002 (12)	0.0010 (12)	0.0031 (12)
C15	0.0198 (15)	0.0117 (13)	0.0153 (13)	0.0008 (11)	−0.0027 (12)	0.0017 (11)
N1	0.0160 (12)	0.0144 (11)	0.0170 (11)	−0.0010 (9)	−0.0006 (10)	0.0000 (10)
N2	0.0222 (12)	0.0136 (12)	0.0226 (12)	−0.0009 (10)	0.0014 (11)	0.0032 (10)
O1	0.0170 (11)	0.0199 (10)	0.0316 (11)	0.0030 (9)	0.0012 (9)	0.0042 (9)
O2	0.0250 (10)	0.0171 (9)	0.0259 (11)	0.0012 (8)	0.0075 (9)	0.0031 (9)

Geometric parameters (Å, º)

C1—C2	1.499 (3)	C9—H9	0.950 (4)
C1—O1	1.319 (3)	C9—N1	1.356 (3)
C1—O2	1.216 (3)	C9—N2	1.313 (3)
C2—C3	1.396 (3)	C10—C11	1.390 (3)
C2—C7	1.405 (3)	C10—C15	1.408 (3)
C3—H3	0.950 (4)	C10—N2	1.388 (3)
C3—C4	1.388 (3)	C11—H11	0.9501 (4)
C4—H4	0.950 (4)	C11—C12	1.385 (4)
C4—C5	1.373 (4)	C12—H12	0.950 (4)
C5—H5	0.950 (4)	C12—C13	1.401 (4)
C5—C6	1.391 (4)	C13—H13	0.950 (4)
C6—H6	0.951 (4)	C13—C14	1.383 (3)
C6—C7	1.389 (4)	C14—H14	0.949 (4)
C7—C8	1.508 (3)	C14—C15	1.391 (4)
C8—H8a	0.990 (4)	C15—N1	1.394 (3)
C8—H8b	0.990 (3)	O1—H1	0.878 (18)
C8—N1	1.469 (3)		
O1—C1—C2	112.3 (2)	N1—C9—H9	123.20 (14)
O2—C1—C2	124.2 (2)	N2—C9—H9	123.20 (15)
O2—C1—O1	123.5 (2)	N2—C9—N1	113.6 (2)
C3—C2—C1	117.7 (2)	C15—C10—C11	121.1 (2)
C7—C2—C1	123.3 (2)	N2—C10—C11	129.7 (2)
C7—C2—C3	118.9 (2)	N2—C10—C15	109.2 (2)
H3—C3—C2	119.23 (15)	H11—C11—C10	121.25 (15)
C4—C3—C2	121.5 (2)	C12—C11—C10	117.5 (3)
C4—C3—H3	119.23 (15)	C12—C11—H11	121.25 (16)
H4—C4—C3	120.26 (15)	H12—C12—C11	119.48 (16)
C5—C4—C3	119.5 (2)	C13—C12—C11	121.0 (2)
C5—C4—H4	120.26 (15)	C13—C12—H12	119.48 (15)
H5—C5—C4	120.16 (15)	H13—C13—C12	118.94 (15)
C6—C5—C4	119.7 (2)	C14—C13—C12	122.1 (2)
C6—C5—H5	120.16 (16)	C14—C13—H13	118.94 (16)
H6—C6—C5	119.13 (16)	H14—C14—C13	121.59 (16)
C7—C6—C5	121.7 (2)	C15—C14—C13	116.8 (3)
C7—C6—H6	119.13 (16)	C15—C14—H14	121.59 (16)

C6—C7—C2	118.6 (2)	C14—C15—C10	121.5 (2)
C8—C7—C2	124.1 (2)	N1—C15—C10	105.3 (2)
C8—C7—C6	117.3 (2)	N1—C15—C14	133.2 (2)
H8a—C8—C7	108.91 (14)	C9—N1—C8	125.7 (2)
H8b—C8—C7	108.91 (13)	C15—N1—C8	127.9 (2)
H8b—C8—H8a	107.7 (3)	C15—N1—C9	106.4 (2)
N1—C8—C7	113.31 (19)	C10—N2—C9	105.4 (2)
N1—C8—H8a	108.91 (12)	H1—O1—C1	111 (2)
N1—C8—H8b	108.91 (12)		
C1—C2—C3—C4	176.5 (2)	C8—N1—C9—N2	−179.6 (2)
C1—C2—C7—C6	−174.8 (2)	C8—N1—C15—C10	179.7 (3)
C1—C2—C7—C8	4.3 (3)	C8—N1—C15—C14	−1.3 (3)
C2—C3—C4—C5	−1.2 (3)	C9—N1—C15—C10	1.0 (2)
C2—C7—C6—C5	−1.9 (3)	C9—N1—C15—C14	179.9 (2)
C2—C7—C8—N1	75.2 (3)	C9—N2—C10—C11	−179.2 (2)
C3—C4—C5—C6	1.8 (3)	C9—N2—C10—C15	0.4 (2)
C4—C5—C6—C7	−0.2 (3)	C10—C11—C12—C13	0.6 (3)
C5—C6—C7—C8	178.9 (2)	C10—C15—C14—C13	0.7 (3)
C6—C7—C8—N1	−105.6 (2)	C11—C12—C13—C14	−0.3 (3)
C7—C8—N1—C9	−116.8 (2)	C12—C13—C14—C15	−0.4 (3)
C7—C8—N1—C15	64.7 (3)	C13—C14—C15—N1	−178.1 (2)

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the N1/N2/C9/C10/C15, C2–C7, C10–C15 and N1/N2/C9–15 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2[i]	0.88 (3)	1.73 (3)	2.592 (3)	164 (4)
C8—H8A···O1[ii]	0.99 (1)	2.62 (1)	3.374 (3)	133 (1)
C3—H3···O1	0.95 (1)	2.28 (1)	2.648 (3)	102 (1)
C8—H8B···O2	0.99 (1)	2.38 (1)	2.846 (3)	108 (1)
C9—H9···O2	0.95 (1)	2.45 (1)	2.861 (3)	106 (1)
C4—H4···*Cg*1[iii]	0.95 (1)	2.99 (1)	3.865 (3)	155 (1)
C4—H4···*Cg*3[iii]	0.95 (1)	2.51 (1)	3.408 (3)	157 (1)
C4—H4···*Cg*4[iii]	0.95 (1)	2.51 (1)	3.454 (3)	170 (1)
C5—H5···*Cg*2[iii]	0.95 (1)	2.76 (1)	3.554 (3)	142 (1)

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