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Crystal structure of serotonin

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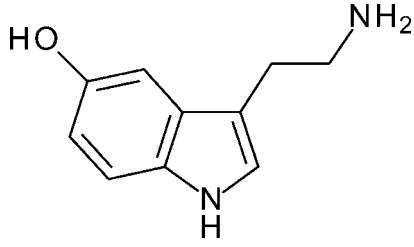
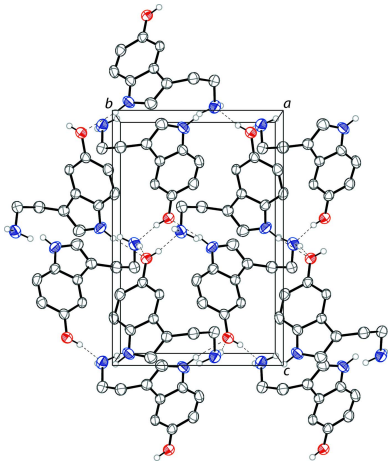
The title compound, serotonin or 5-hydroxytryptamine (5-HT) [systematic name: 3-(2-aminoethyl)-1*H*-indol-5-ol], $C_{10}H_{12}N_2O$, has one molecule in the asymmetric unit. The conformation of the ethylamino side chain is *gauche*–*gauche* [$C_a-C_a-C_m-C_m$ and $C_a-C_m-C_m-N$ (a = aromatic, m = methylene) torsion angles = −64.2 (3) and −61.9 (2)°, respectively]. In the crystal, the molecules are linked into a three-dimensional network by N—H···O and O—H···N hydrogen bonds.

1. Chemical context

Serotonin, $C_{10}H_{12}N_2O$, systematic name 3-(2-aminoethyl)-1*H*-indol-5-ol, is the primary neurotransmitter in humans, regulating mood, anxiety and happiness (Young & Leyton, 2002). While it is best known for its role in the central nervous system, serotonin is found throughout the human body and impacts a wide array of bodily functions. Roughly ninety-five percent of the body's serotonin is actually found in the gastrointestinal tract, where it regulates intestinal movement (Berger *et al.*, 2009). Serotonin is produced in the human body through biosynthesis from the essential amino acid tryptophan (Fitzpatrick, 1999), and broken down by monoamine oxidase to generate 5-hydroxyindoleacetic acid. As such, monoamine oxidase inhibitors and other compounds that increase serotonin concentration have been used to treat depression (Suchting *et al.*, 2021).



Serotonin is not unique to humans, but is found throughout life on Earth including all bilateral animals, where it also functions as a neurotransmitter (Bacqué-Cazenave *et al.*, 2020). It is found in plants, notably in seeds, where serotonin stimulates the digestive tract of animals, leading to excretion of the seeds (Akula *et al.*, 2011). Serotonin and related tryptamines are well known to be present in a number of fungi (Tyler, 1958; Sherwood *et al.*, 2020). A variety of related tryptamines found in plants, fungi, and toads, which are active at serotonin receptors, have garnered significant attention as psychedelic drugs to treat mood disorders including anxiety, depression, and addiction (Carhart-Harris & Goodwin, 2017). Serotonin was discovered by Vittorio Erspaner in 1935,



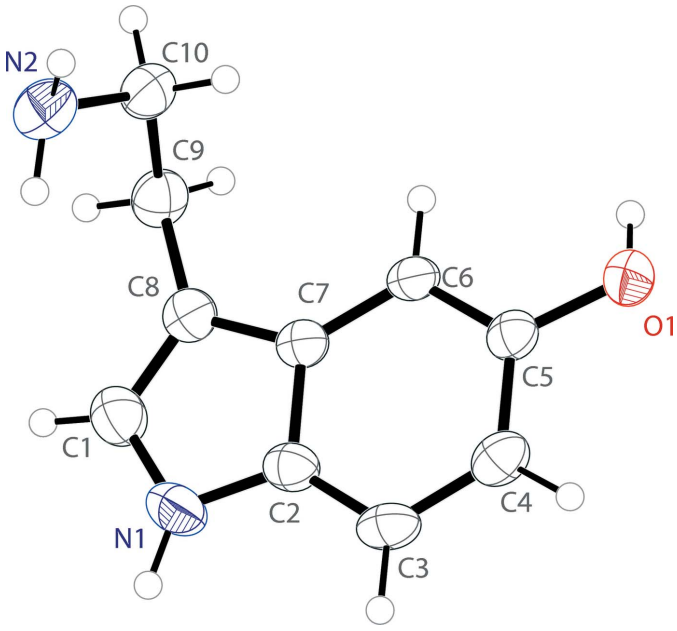


Figure 1
The molecular structure of serotonin free base showing the atomic labeling. Displacement ellipsoids are drawn at the 50% probability level.

characterized as 5-hydroxytryptamine (5-HT) in 1949 by Rapport, and synthesized by Upjohn pharmaceutical in 1951 (Whitaker-Azmitia, 1999). Despite the simplicity of its structure and universally recognized biological significance, the single-crystal structure of pure free base serotonin has never been reported. Herein, we report this structure to fill in the gap from the scientific record.

2. Structural commentary

Serotonin or 5-hydroxytryptamine (5-HT) is an indolamine with a 5-hydroxy substitution. In the solid state, serotonin crystallizes with one molecule in the asymmetric unit (Fig. 1) in the chiral space group $P2_12_12_1$. The 5-hydroxyindole fused-ring unit is almost planar with the non-hydrogen atoms showing an r.m.s. deviation from planarity of 0.030 Å. The ethylamino arm is turned away from the indole ring, with a C7—C8—C9—C10 torsion angle of −64.2 (3)°. The ethylamino arm itself turns back toward the indole ring with a C8—C9—C10—N2 torsion angle of −61.9 (2)°.

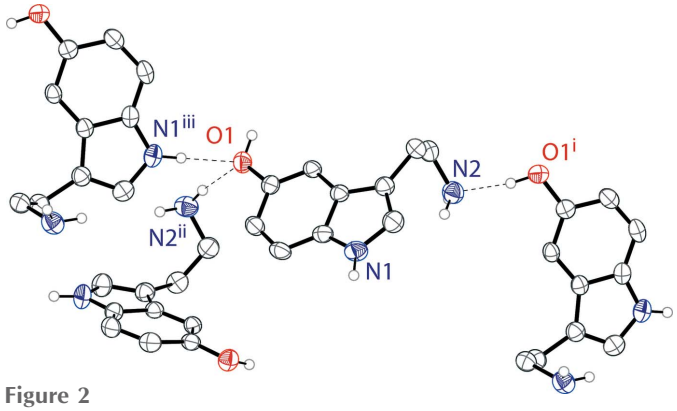


Figure 2
The different hydrogen-bonding interactions between the serotonin molecules. Hydrogen atoms not involved in hydrogen bonding are omitted for clarity. Symmetry codes: (i) $\frac{3}{2}-x, 1-y, \frac{1}{2}+z$ (ii) $2-x, -\frac{1}{2}+y, \frac{1}{2}-z$ (iii) 3/2 − x, −y, $-\frac{1}{2}+z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2^{i}	0.88 (1)	1.77 (1)	2.636 (2)	170 (3)
N1—H1A···O1^{ii}	0.88 (1)	2.10 (1)	2.967 (2)	169 (2)
N2—H2B···O1^{iii}	0.91 (1)	2.19 (1)	3.092 (3)	168 (2)

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

3. Supramolecular features

In the crystal, the serotonin molecules are linked by a series of hydrogen bonds that produce a three-dimensional network in the solid state. The hydroxy groups form hydrogen bonds to the amine N atoms on an adjacent serotonin molecules forming O1—H1···N2 hydrogen bonds. The indole N atoms form hydrogen bonds to the hydroxy groups of adjacent serotonin molecules through N1—H1A···O1 hydrogen bonds. Half of the amine H atoms link to the hydroxy groups of nearby molecules through N2—H2B···O1 hydrogen bonds. There are no observed π–π stacking interactions. Fig. 2

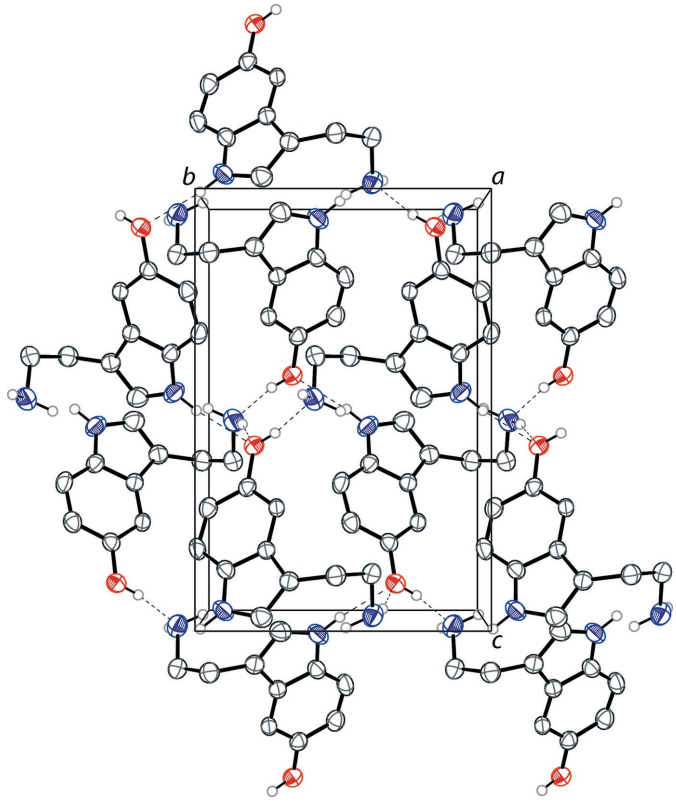


Figure 3
The crystal packing of serotonin free base viewed along the a-axis. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonds are omitted for clarity.

Table 2
Torsion angles of the ethylamino arms of different serotonin structures (our atom-numbering scheme).

	Space group	C7—C8—C9—C10	C8—C9—C10—N2	Reference
5-HT free base	$P2_12_12_1$	−64.2 (3)	−61.9 (2)	This work
HTRCRS	$C2/c$	166.7	172.6	Karle *et al.* (1965)
SERHOX	$P2_1/n$	171.7	179.7	Amit *et al.* (1978)
SERPIC	$P2_1/c$	67.5	66.6	Thewalt & Bugg (1972)
VIKWIX	$P\overline{1}$	178.7	177.2	Rychkov *et al.* (2013)
RAWDIF	$Pca2_1$	177.8	177.6	Feng *et al.* (2017)
RAWDO*L*[a]	Cc	178.7	175.1	Feng *et al.* (2017)
RAWDO*L*[b]	Cc	102	43	Feng *et al.* (2017)

Notes: (*a*, *b*) RAWDOL contains two molecules in the asymmetric unit. The *b* molecule is probably disordered and the geometrical data are less certain.

outlines the hydrogen bonds, which are detailed in Table 1. The crystal packing of serotonin is shown in Fig. 3.

4. Database survey

The previous structural reports of serotonin are all complex mixtures containing serotonin in its $C_{10}H_{13}N_2O^+$ cationic form. These include the creatine sulfate monohydrate (Karle *et al.*, 1965: Cambridge Structural Database refcode HTRCRS), the hydrogen oxalate salt (Amit *et al.*, 1978: SERHOX), the hydroadipate salt (Rychkov *et al.*, 2013: VIKWIX), the picrate monohydrate (Thewalt & Bugg, 1972: SERPIC) and two compounds where it is co-crystallized with 1,3,6,8-tetrasulfonatopyrene (Feng *et al.*, 2017: RAWDIF, RAWDOL). The two most closely reported free-base structures to serotonin are the natural product bufotenine, 5-hydroxy-*N*,*N*-dimethyltryptamine (Falkenberg, 1972: BUFTEN) and 5-methoxytryptamine (Quarles *et al.*, 1974: MXTRYP). 5-Methoxytryptamine has also been reported as its picrate (Nagata *et al.*, 1995: ZILMIQ) and chloride (Pham *et al.*, 2021: CCDC 2106050) salts. The free base reported here shows the ethylamino arm turned away from the indole plane. The majority of the cationic tryptamine structures show ethylamino arms that are nearly in-plane with the indole ring. Only the picrate salt has a structure similar to that of the title compound, showing an ethylamino arm turned similarly away from the indole ring. The torsion angles associated with the ethylamino arms of the different structures are summarized in Table 2.

5. Synthesis and crystallization

Single crystals suitable for X-ray diffraction studies were grown from the slow evaporation of a tetrahydrofuran solution of a commercial sample of serotonin free base (Chem-Impex).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms H1, H1*A*, H2*A* and H2*B* were found from a difference-Fourier map and were refined isotropically, using DFIX restraints with an N—H(indole) distance of 0.87 (1) Å, N—H(amine) distances of 0.90 (1) Å, and an O—H distance of 0.86 (1) Å. Isotropic displacement parameters were set to 1.2 U_{eq} of the parent nitrogen atoms and 1.5 U_{eq} of the parent oxygen atom. All other hydrogen atoms were placed in calculated positions with C—H = 0.93 Å (sp^2) or 0.97 Å (sp^3). Isotropic displacement parameters were set to 1.2 U_{eq} of the parent carbon atoms. The absolute structure of the crystal chosen for data collection was indeterminate in the present refinement.

Acknowledgements

Financial statements and conflict of interest: This study was funded by CaaMTech, Inc. ARC reports an ownership interest

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{12}N_2O$
M_r	176.22
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	297
a, b, c (Å)	8.2248 (6), 8.7542 (6), 13.0712 (10)
V (Å^3)	941.15 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.18 × 0.10 × 0.02
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2018)
T_{min}, T_{max}	0.711, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25138, 1783, 1590
R_{int}	0.052
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.073, 1.05
No. of reflections	1783
No. of parameters	134
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.13, −0.13
Absolute structure	Flack x determined using 609 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−1.2 (6)

Computer programs: *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2018), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *publCIF* (Westrip, 2010).

in CaaMTech, Inc., which owns US and worldwide patent applications, covering new tryptamine compounds, compositions, formulations, novel crystalline forms, and methods of making and using the same.

Funding information

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Computing details

Data collection: *APEX3* (Bruker, 2018); cell refinement: *SAINT* (Bruker, 2018); data reduction: *SAINT* (Bruker, 2018); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

3-(2-Aminoethyl)-1*H*-indol-5-ol

Crystal data

$C_{10}H_{12}N_2O$
M_r = 176.22
Orthorhombic, $P2_12_12_1$
a = 8.2248 (6) Å
b = 8.7542 (6) Å
c = 13.0712 (10) Å
V = 941.15 (12) Å^3
Z = 4
$F(000)$ = 376
D_x = 1.244 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6263 reflections
θ = 3.1–25.4°
μ = 0.08 mm^{-1}
T = 297 K
Block, colourless
0.18 × 0.10 × 0.02 mm

Data collection

Bruker D8 Venture CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2018)
T_{min} = 0.711, T_{max} = 0.745
25138 measured reflections
1783 independent reflections
1590 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 25.7°, θ_{min} = 2.8°
h = −10→10
k = −10→10
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.073
S = 1.05
1783 reflections
134 parameters
4 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 0.1115P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Absolute structure: Flack x determined using 609 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −1.2 (6)

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}
O1	0.91964 (18)	0.18734 (16)	0.08462 (10)	0.0398 (4)
H1	0.868 (3)	0.263 (2)	0.054 (2)	0.078 (9)*
N1	0.6390 (2)	0.0903 (2)	0.45983 (14)	0.0445 (5)
H1A	0.633 (3)	0.012 (2)	0.5016 (15)	0.051 (7)*
N2	0.7279 (2)	0.6020 (2)	0.47447 (15)	0.0458 (5)
H2A	0.725 (3)	0.5092 (18)	0.5030 (18)	0.050 (7)*
H2B	0.8312 (19)	0.638 (3)	0.465 (2)	0.072 (9)*
C1	0.5533 (3)	0.2238 (2)	0.47087 (16)	0.0433 (5)
H1B	0.487070	0.246998	0.526412	0.052*
C2	0.7237 (2)	0.0960 (2)	0.36910 (15)	0.0343 (4)
C3	0.8303 (2)	−0.0077 (2)	0.32446 (16)	0.0388 (5)
H3	0.856712	−0.098830	0.357097	0.047*
C4	0.8956 (2)	0.0283 (2)	0.23057 (16)	0.0375 (5)
H4	0.967797	−0.039127	0.199600	0.045*
C5	0.8552 (2)	0.1654 (2)	0.18068 (14)	0.0316 (4)
C6	0.7543 (2)	0.27075 (19)	0.22632 (14)	0.0304 (4)
H6	0.731045	0.362796	0.193965	0.036*
C7	0.6874 (2)	0.2373 (2)	0.32214 (14)	0.0300 (4)
C8	0.5785 (2)	0.3173 (2)	0.38953 (14)	0.0349 (4)
C9	0.5130 (2)	0.4756 (2)	0.37352 (17)	0.0391 (5)
H9A	0.434413	0.497950	0.426806	0.047*
H9B	0.456668	0.479381	0.308368	0.047*
C10	0.6446 (3)	0.5971 (2)	0.37477 (16)	0.0412 (5)
H10A	0.723268	0.575700	0.321372	0.049*
H10B	0.596386	0.696063	0.360712	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0473 (8)	0.0370 (8)	0.0351 (7)	0.0049 (7)	0.0058 (6)	−0.0021 (6)
N1	0.0536 (11)	0.0411 (10)	0.0390 (10)	0.0009 (9)	0.0040 (9)	0.0125 (8)
N2	0.0465 (11)	0.0406 (10)	0.0502 (12)	0.0012 (9)	−0.0064 (9)	−0.0055 (9)
C1	0.0441 (11)	0.0456 (13)	0.0402 (11)	0.0009 (10)	0.0064 (9)	0.0025 (9)
C2	0.0378 (10)	0.0309 (9)	0.0342 (10)	−0.0019 (8)	−0.0068 (9)	0.0044 (8)
C3	0.0434 (11)	0.0268 (9)	0.0461 (11)	0.0031 (8)	−0.0094 (10)	0.0058 (8)
C4	0.0366 (10)	0.0325 (10)	0.0435 (11)	0.0061 (8)	−0.0055 (9)	−0.0036 (9)
C5	0.0322 (9)	0.0299 (9)	0.0328 (9)	−0.0033 (7)	−0.0037 (8)	−0.0034 (8)
C6	0.0360 (9)	0.0230 (8)	0.0323 (9)	−0.0004 (8)	−0.0052 (8)	0.0010 (7)
C7	0.0304 (9)	0.0282 (9)	0.0315 (9)	−0.0012 (7)	−0.0060 (7)	0.0001 (7)

C8	0.0348 (9)	0.0347 (10)	0.0353 (10)	0.0004 (8)	−0.0024 (9)	−0.0004 (8)
C9	0.0377 (10)	0.0390 (11)	0.0406 (11)	0.0078 (9)	−0.0006 (9)	−0.0009 (9)
C10	0.0493 (12)	0.0340 (10)	0.0404 (11)	0.0045 (9)	−0.0001 (10)	−0.0030 (9)

Geometric parameters (Å, º)

O1—H1	0.878 (13)	C3—C4	1.376 (3)
O1—C5	1.376 (2)	C4—H4	0.9300
N1—H1A	0.879 (12)	C4—C5	1.406 (3)
N1—C1	1.373 (3)	C5—C6	1.376 (3)
N1—C2	1.376 (3)	C6—H6	0.9300
N2—H2A	0.894 (12)	C6—C7	1.399 (3)
N2—H2B	0.914 (13)	C7—C8	1.438 (3)
N2—C10	1.473 (3)	C8—C9	1.501 (3)
C1—H1B	0.9300	C9—H9A	0.9700
C1—C8	1.358 (3)	C9—H9B	0.9700
C2—C3	1.391 (3)	C9—C10	1.518 (3)
C2—C7	1.412 (3)	C10—H10A	0.9700
C3—H3	0.9300	C10—H10B	0.9700
C5—O1—H1	109.1 (19)	C5—C6—H6	120.5
C1—N1—H1A	124.8 (16)	C5—C6—C7	119.01 (16)
C1—N1—C2	108.64 (16)	C7—C6—H6	120.5
C2—N1—H1A	126.4 (16)	C2—C7—C8	107.00 (17)
H2A—N2—H2B	113 (2)	C6—C7—C2	119.27 (17)
C10—N2—H2A	109.3 (16)	C6—C7—C8	133.72 (17)
C10—N2—H2B	108.5 (18)	C1—C8—C7	106.30 (17)
N1—C1—H1B	124.7	C1—C8—C9	127.65 (19)
C8—C1—N1	110.65 (19)	C7—C8—C9	126.01 (17)
C8—C1—H1B	124.7	C8—C9—H9A	109.0
N1—C2—C3	131.04 (18)	C8—C9—H9B	109.0
N1—C2—C7	107.41 (16)	C8—C9—C10	112.92 (16)
C3—C2—C7	121.54 (18)	H9A—C9—H9B	107.8
C2—C3—H3	121.0	C10—C9—H9A	109.0
C4—C3—C2	118.04 (17)	C10—C9—H9B	109.0
C4—C3—H3	121.0	N2—C10—C9	111.17 (17)
C3—C4—H4	119.4	N2—C10—H10A	109.4
C3—C4—C5	121.14 (18)	N2—C10—H10B	109.4
C5—C4—H4	119.4	C9—C10—H10A	109.4
O1—C5—C4	116.80 (17)	C9—C10—H10B	109.4
C6—C5—O1	122.29 (17)	H10A—C10—H10B	108.0
C6—C5—C4	120.90 (17)		
O1—C5—C6—C7	177.03 (16)	C3—C2—C7—C6	2.9 (3)
N1—C1—C8—C7	0.2 (2)	C3—C2—C7—C8	−178.28 (17)
N1—C1—C8—C9	−177.44 (19)	C3—C4—C5—O1	−176.50 (17)
N1—C2—C3—C4	178.8 (2)	C3—C4—C5—C6	2.8 (3)
N1—C2—C7—C6	−178.03 (16)	C4—C5—C6—C7	−2.3 (3)

N1—C2—C7—C8	0.8 (2)	C5—C6—C7—C2	−0.5 (2)
C1—N1—C2—C3	178.3 (2)	C5—C6—C7—C8	−178.96 (18)
C1—N1—C2—C7	−0.7 (2)	C6—C7—C8—C1	178.0 (2)
C1—C8—C9—C10	113.0 (2)	C6—C7—C8—C9	−4.4 (3)
C2—N1—C1—C8	0.3 (3)	C7—C2—C3—C4	−2.4 (3)
C2—C3—C4—C5	−0.5 (3)	C7—C8—C9—C10	−64.2 (3)
C2—C7—C8—C1	−0.6 (2)	C8—C9—C10—N2	−61.9 (2)
C2—C7—C8—C9	177.08 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	0.88 (1)	1.77 (1)	2.636 (2)	170 (3)
N1—H1*A*···O1^{ii}	0.88 (1)	2.10 (1)	2.967 (2)	169 (2)
N2—H2*B*···O1^{iii}	0.91 (1)	2.19 (1)	3.092 (3)	168 (2)

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