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4-Hydroxy-*N,N*-diisopropyltryptammonium hydrofumarate

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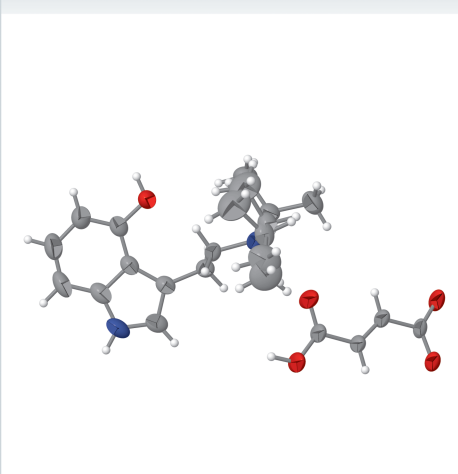
Keywords: crystal structure; tryptamines; indoles; hydrogen bonding.

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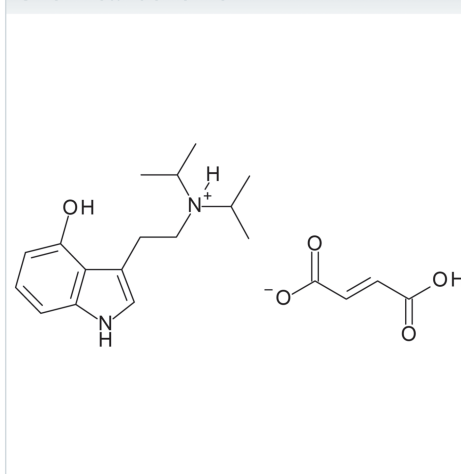
Structural data: full structural data are available from iucrdata.iucr.org

The solid-state structure of the title salt, $C_{16}H_{25}N_2O^+ \cdot C_4H_3O_4^-$ [systematic name: [2-(4-hydroxy-1*H*-indol-3-yl)ethyl]bis(propan-2-yl)azanium (2*E*)-3-carboxyprop-2-enoate], is reported. In the extended structure, the hydrofumarate anions form linear chains propagating in the [100] direction through O—H...O hydrogen bonds that combine with the tryptammonium cations to generate a three-dimensional network linked by O—H...O and N—H...O hydrogen bonds.

3D view



Chemical scheme



Structure description

4-Hydroxy-*N,N*-diisopropyltryptamine (4-HO-DiPT, $C_{16}H_{24}N_2O$) is a synthetic structural analog of serotonin (5-hydroxytryptamine), which differs by moving the hydroxy moiety from the 5- to the 4- position of the indole unit, and di-alkylating its primary amine with two isopropyl groups. Serotonin analogs have been the subject of fascination for millenia because they alter human perception and consciousness when ingested (George *et al.*, 2022), effects now attributed to the 5-HT_{2A} receptor (Halberstadt & Geyer, 2011). Psilocybin (4-phosphoryloxy-*N,N*-dimethyltryptamine) and psilocin (4-hydroxy-*N,N*-dimethyltryptamine) are widely known examples, both natural products found in at least 200 species of so-called ‘magic’ mushrooms (Nichols, 2020). Other naturally occurring serotonin analogs (*e.g.* 5-MeO-DMT, DMT, bufotenine) have been identified in plants and animals (Araújo *et al.*, 2015). Different structural analogs of serotonin produce varied perceptual and biological effects in humans.

Recently, several studies have indicated that 5-HT_{2A} agonists hold tremendous potential to treat the most harmful and intractable mental health conditions including depression, anxiety and post-traumatic stress disorder (PTSD). Psilocybin and other psilocin prodrugs are currently being developed as a treatment for treatment-resistant depression (TRD), anorexia and PTSD (Goodwin *et al.*, 2022). 5-Methoxy-*N,N*-dimethyltryptamine (5-MeO-DMT) is also in Phase 2 trials as treatment for TRD



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(Reckweg *et al.*, 2023). A prodrug of the title compound is in Phase 2 clinical trials for the treatment of post partem depression and adjustment disorder (NIH, 2025).

Alongside these clinical studies, others have sought to elucidate a structure–activity relationship (SAR), by understanding how the structural differences across serotonin analogs correlate with their pharmacological and, ultimately, clinical differences in human subjects. 4-Hydroxy-*N,N*-diisopropyltryptamine (4-HO-DiPT) was first synthesized in 1977 as its hydrochloride salt (Repke *et al.*, 1977). This sterically bulky analogue of psilocin is more selective toward serotonin receptors, binding to three of the possible 14 receptors, while psilocin and less bulky analogues often bind to ten (Glatfelter *et al.*, 2023). This synthetic variant of psilocin has been noted for its fast onset, brevity and intensity of action (Shulgin & Shulgin, 2016).

In 2022, the US Drug Enforcement Agency proposed reclassifying 4-HO-DiPT to Schedule I of the Controlled Substance Act; the proposal was withdrawn due to strong public response (US DEA, January 14 and July 6, 2022*a,b*). Alongside this proposed rescheduling of 4-HO-DiPT, Reunion Neuroscience (Toronto, Canada) initiated clinical trials of a ‘hemi-ester’ prodrug of the same, *i.e.* 4-glutarato-*N,N*-diisopropyltryptamine. We have published ethanol and methanol solvates of this prodrug, which are the first two crystal structures of this compound, and also the first structures of any *N,N*-diisopropyltryptamine (Naeem *et al.*, 2022). The propensity of this prodrug to form solvates in the solid state could potentially explain the difficulties removing impurities described in the later report on the synthesis and activity of this compound (Bryson *et al.*, 2024). While we have reported the first crystal structures of these prodrugs, the structure of the active metabolite has been absent. Herein, we report the first crystal structure of 4-hydroxy-*N,N*-diisopropyltryptamine as its hydrofumarate salt.

The molecular structure of the title compound is shown in Fig. 1. The asymmetric unit contains one 4-hydroxy-*N,N*-diisopropyltryptammonium ($C_{16}H_{25}N_2O^+$) cation and one

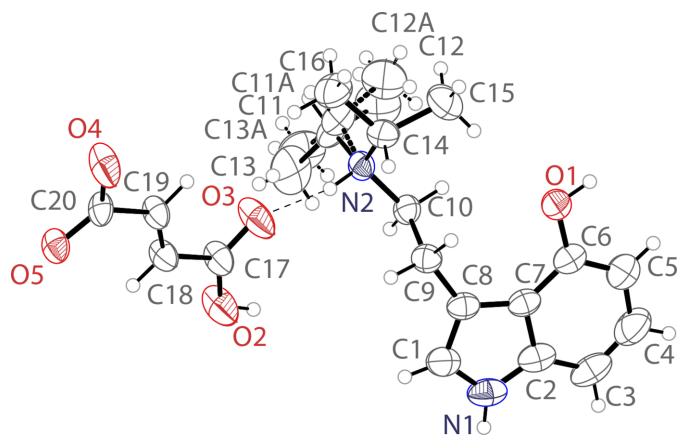


Figure 1

The molecular structure of the title compound showing the atomic labeling. Displacement ellipsoids are drawn at the 50% probability level. Dashed bonds indicate a disordered component in the structure. Hydrogen bonds are shown as dashed lines.

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2A\cdots O4^i$	0.91 (1)	1.54 (2)	2.441 (3)	173 (6)
$N1-H1A\cdots O5^{ii}$	0.87 (1)	2.13 (2)	2.989 (3)	170 (4)
$N2-H2\cdots O3$	0.90 (1)	1.88 (1)	2.756 (3)	165 (2)
$O1-H1\cdots O5^{iii}$	0.89 (1)	1.89 (1)	2.784 (3)	177 (4)

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

hydrofumarate ($C_4H_3O_4^-$) anion. The indole ring of the cation is near planar with a r.m.s. deviation from planarity of 0.005 Å for the non-hydrogen atoms. The hydrofumarate anion is slightly less planar with a r.m.s. deviation from planarity of 0.081 Å for the non-hydrogen atoms. The ethyl-amino arm of the tryptamine is turned away from the indole plane with a $C7-C8-C9-C10$ torsion angle of 75.9 (3)° and the $C8-C9-C10-N2$ grouping has an *anti* conformation [torsion angle = 170.4 (2)°]. One of the isopropyl groups ($C11-C13$) is disordered over two orientations in a 0.51 (4):0.49 (4) ratio. In the extended structure, the hydrofumarate anions form linear chains along [100] through $O-H\cdots O$ hydrogen bonds (Table 1, Fig. 2). These chains are connected into a three-dimensional network by $O-H\cdots O$ and $N-H\cdots O$ hydrogen bonds with the tryptammonium cations.

In addition to the structure reported here, there are eight other hydrofumarate salts of tryptamines reported including those of *N*-ethyl-*N*-*n*-propyltryptamine (Cambridge Structural

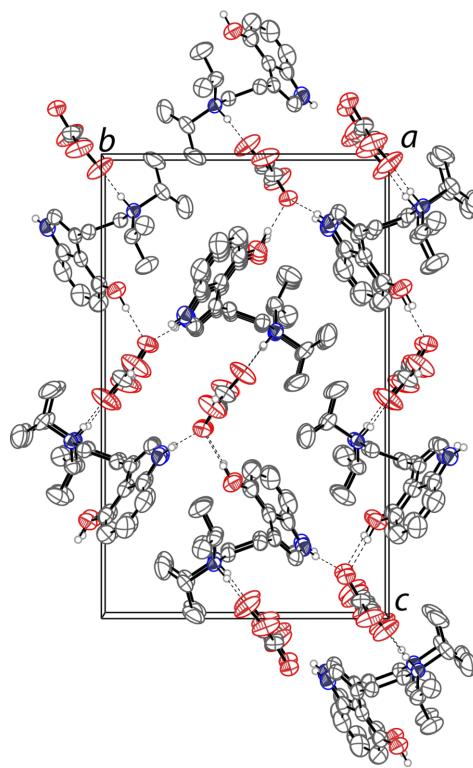


Figure 2

The crystal packing of the title compound viewed along the *a* axis. The hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonds are omitted for clarity. Only one component of the disordered isopropyl groups are shown.

Database refcode GUPBOL; Chadeayne *et al.*, 2020c) and *N*-allyl-*N*-methyltryptamine (GUPBUR; Chadeayne *et al.*, 2020c), 4-acetoxy-*N,N*-dimethyltryptamine (HOCJUH; Chadeayne *et al.*, 2019a), 4-acetoxy-*N*-ethyl-*N*-methyltryptamine (OJIIQIK; Pham *et al.*, 2021a) and 4-acetoxy-*N*-allyl-*N*-methyltryptamine (OJIIQUQ; Pham *et al.*, 2021a), *N*-methyl-*N*-isopropyltryptamine (RONSOFF; Chadeayne *et al.*, 2019c) and 4-hydroxy-*N*-methyl-*N*-isopropyltryptamine (RONSUL; Chadeayne *et al.*, 2019c), and 4-propionoxy-*N,N*-dimethyltryptamine (Glatfelter *et al.*, 2023). The other tryptamine structures reported with fumaric acid based counterions are nine (2:1) tryptamine:fumarate salts including those of the anti-cancer drug panobinostat (MIMMAA; Kenguva *et al.*, 2023), the mushroom natural product norpsilocin (MULXEZ; Chadeayne *et al.*, 2020b), 5-methoxy-*N,N*-diallyltryptamine (OPUDEL; Pham *et al.*, 2021c), 5-methoxy-*N,N*-di-*n*-propyltryptamine (OQIGON; Pham *et al.*, 2021d), 4-hydroxy-*N*-methyl-*N*-isopropyltryptamine (TUFQAP; Chadeayne *et al.*, 2020a), 5-methoxy-2-methyl-*N,N*-dimethyltryptamine (ULUTED; Pham *et al.*, 2021b), 4-hydroxy-*N,N*-di-*n*-propyltryptamine (WUCGAF; Chadeayne *et al.*, 2019d), psilocetin (XOFDOO; Chadeayne *et al.*, 2019b), *N*-cyclohexyltryptamine (YITWIL; Naeem *et al.*, 2023), and two (2:1:1) tryptamine:fumarate:fumaric acid complexes, being those of 4-acetoxy-*N*-ethyl-*N*-*n*-propyltryptamine (BIYKED; Pham *et al.*, 2023) and 4-acetoxy-*N,N*-diallyltryptamine (OJIIQUW; Pham *et al.*, 2021a). There are also two structures of the 4-HO-DiPT prodrug 4-glutarato-*N,N*-diisopropyltryptamine reported (TEKWOZ, TEKWUF; Naeem *et al.*, 2022).

Synthesis and crystallization

Slow evaporation of a methanol/water solution of a commercial sample of '4-HO-DiPT fumarate' (Chem Logix) resulted in the formation of colorless blocks of the title compound suitable for X-ray analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C11–C13 isopropyl group is disordered over two orientations in a 0.51 (4):0.49 (4) ratio. The disorder model was restrained with N–C distances of 1.50 (1) Å, as well as SADI C–C distance restraints, DELU rigid body restraints, and ISOR isotropic restraints. The structure was refined as an inversion twin.

Acknowledgements

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

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₆ H ₂₅ N ₂ O ⁺ ·C ₄ H ₃ O ₄ [−]
<i>M_r</i>	376.44
Crystal system, space group	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁
Temperature (K)	300
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.9541 (3), 12.5763 (5), 20.3351 (6)
<i>V</i> (Å ³)	2034.18 (13)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
<i>μ</i> (mm ^{−1})	0.09
Crystal size (mm)	0.38 × 0.24 × 0.12
Data collection	
Diffractionmeter	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.714, 0.745
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	23480, 3864, 3485
<i>R_{int}</i>	0.034
(sin θ/λ) _{max} (Å ^{−1})	0.611
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.039, 0.095, 1.08
No. of reflections	3864
No. of parameters	295
No. of restraints	54
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.14, −0.12
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.6 (15)

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

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full crystallographic data

IUCrData (2025). **10**, x250564 [https://doi.org/10.1107/S2414314625005644]

4-Hydroxy-*N,N*-diisopropyltryptammonium hydrofumarate

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[2-(4-Hydroxy-1*H*-indol-3-yl)ethyl]bis(propan-2-yl)azanium (2*E*)-3-carboxyprop-2-enoate

Crystal data

$C_{16}H_{25}N_2O^+ \cdot C_4H_3O_4^-$

$M_r = 376.44$

Orthorhombic, $P2_12_12_1$

$a = 7.9541$ (3) Å

$b = 12.5763$ (5) Å

$c = 20.3351$ (6) Å

$V = 2034.18$ (13) Å³

$Z = 4$

$F(000) = 808$

$D_x = 1.229$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9289 reflections

$\theta = 2.8$ – 25.6°

$\mu = 0.09$ mm⁻¹

$T = 300$ K

Block, colourless

$0.38 \times 0.24 \times 0.12$ mm

Data collection

Bruker D8 Venture CMOS
diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.714$, $T_{\max} = 0.745$

23480 measured reflections

3864 independent reflections

3485 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 25.7^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -9 \rightarrow 9$

$k = -15 \rightarrow 15$

$l = -18 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.095$

$S = 1.08$

3864 reflections

295 parameters

54 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.3705P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.14$ e Å⁻³

$\Delta\rho_{\min} = -0.12$ e Å⁻³

Absolute structure: Refined as an inversion twin

Absolute structure parameter: 0.6 (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. Atoms H1, H1A, H2, and H2A were found from difference-Fourier maps and allowed to refine with restrained an N—H distance of 0.87 (1) Å and 1.20 U_{eq} of the parent indole nitrogen, an N—H distance 0.90 (1) Å and 1.20 U_{eq} of the parent ammonium nitrogen, and O—H distances of 0.90 (1) Å and 1.50 U_{eq} of parent oxygen atoms. All other hydrogen atoms were placed in calculated positions with appropriate riding parameters. Refined as a 2-component inversion twin.

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

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}	Occ. (<1)
O1	0.7205 (3)	0.45612 (17)	0.21046 (10)	0.0586 (5)	
O2	0.3240 (2)	0.6148 (2)	0.54461 (13)	0.0875 (9)	
H2A	0.427 (3)	0.602 (4)	0.527 (3)	0.16 (2)*	
O3	0.2145 (2)	0.5076 (2)	0.47141 (12)	0.0839 (8)	
O4	−0.3942 (2)	0.5705 (2)	0.50563 (10)	0.0791 (8)	
O5	−0.2902 (2)	0.65068 (16)	0.59369 (8)	0.0486 (4)	
N1	0.9479 (3)	0.7045 (2)	0.35061 (13)	0.0586 (7)	
N2	0.3986 (3)	0.39208 (16)	0.38155 (10)	0.0406 (5)	
C1	0.7910 (4)	0.6762 (2)	0.37158 (14)	0.0531 (7)	
H1B	0.738117	0.703461	0.408711	0.064*	
C2	0.9858 (3)	0.6496 (2)	0.29497 (14)	0.0518 (7)	
C3	1.1308 (4)	0.6528 (3)	0.25608 (19)	0.0673 (9)	
H3	1.221446	0.696320	0.266611	0.081*	
C4	1.1325 (4)	0.5891 (3)	0.2022 (2)	0.0764 (10)	
H4	1.227306	0.589094	0.175423	0.092*	
C5	0.9968 (4)	0.5233 (3)	0.18541 (17)	0.0689 (9)	
H5	1.003159	0.481506	0.147773	0.083*	
C6	0.8555 (4)	0.5198 (2)	0.22348 (15)	0.0514 (7)	
C7	0.8470 (3)	0.58421 (19)	0.28019 (13)	0.0435 (6)	
C8	0.7230 (3)	0.60230 (19)	0.33038 (12)	0.0440 (6)	
C9	0.5517 (3)	0.5530 (2)	0.33740 (13)	0.0440 (6)	
H9A	0.495522	0.553065	0.295076	0.053*	
H9B	0.484818	0.595014	0.367676	0.053*	
C10	0.5650 (3)	0.4400 (2)	0.36269 (12)	0.0411 (5)	
H10A	0.616347	0.396122	0.328976	0.049*	
H10B	0.638543	0.439132	0.400747	0.049*	
C11	0.427 (2)	0.2918 (10)	0.4237 (8)	0.052 (3)	0.49 (4)
H11	0.318518	0.255912	0.428418	0.062*	0.49 (4)
C12	0.547 (3)	0.2139 (15)	0.3918 (12)	0.101 (5)	0.49 (4)
H12A	0.533434	0.145121	0.411493	0.151*	0.49 (4)
H12B	0.660493	0.237862	0.397948	0.151*	0.49 (4)
H12C	0.522964	0.209468	0.345594	0.151*	0.49 (4)
C13	0.488 (3)	0.320 (2)	0.4921 (8)	0.092 (5)	0.49 (4)
H13A	0.404651	0.362825	0.513684	0.138*	0.49 (4)
H13B	0.591273	0.358873	0.489015	0.138*	0.49 (4)
H13C	0.505785	0.255956	0.516831	0.138*	0.49 (4)
C11A	0.402 (2)	0.2809 (8)	0.4102 (8)	0.054 (3)	0.51 (4)
H11A	0.284595	0.259997	0.417814	0.065*	0.51 (4)
C12A	0.479 (3)	0.1967 (11)	0.3682 (11)	0.096 (5)	0.51 (4)

H12D	0.493440	0.132917	0.393531	0.144*	0.51 (4)
H12E	0.586697	0.220607	0.352648	0.144*	0.51 (4)
H12F	0.407206	0.182372	0.331322	0.144*	0.51 (4)
C13A	0.484 (3)	0.2892 (16)	0.4766 (11)	0.091 (4)	0.51 (4)
H13D	0.474229	0.222598	0.499337	0.137*	0.51 (4)
H13E	0.430600	0.344092	0.501814	0.137*	0.51 (4)
H13F	0.601223	0.306291	0.471114	0.137*	0.51 (4)
C14	0.2691 (4)	0.3954 (2)	0.32555 (13)	0.0512 (7)	
H14	0.250591	0.470741	0.315689	0.061*	
C15	0.3301 (5)	0.3449 (3)	0.26212 (17)	0.0861 (12)	
H15A	0.436477	0.375199	0.250051	0.129*	
H15B	0.249718	0.357998	0.227835	0.129*	
H15C	0.342555	0.269678	0.268344	0.129*	
C16	0.1007 (4)	0.3515 (3)	0.34731 (17)	0.0685 (8)	
H16A	0.069079	0.383492	0.388358	0.103*	
H16B	0.109015	0.275878	0.352725	0.103*	
H16C	0.017280	0.367423	0.314643	0.103*	
C17	0.2024 (3)	0.5696 (3)	0.51642 (13)	0.0529 (7)	
C18	0.0350 (3)	0.5989 (2)	0.54360 (14)	0.0507 (7)	
H18	0.030972	0.640540	0.581360	0.061*	
C19	−0.1049 (3)	0.5692 (2)	0.51722 (12)	0.0454 (6)	
H19	−0.099546	0.525415	0.480425	0.055*	
C20	−0.2747 (3)	0.6005 (2)	0.54185 (12)	0.0437 (6)	
H1A	1.015 (4)	0.749 (2)	0.3704 (16)	0.093 (13)*	
H2	0.355 (3)	0.4362 (17)	0.4119 (10)	0.040 (7)*	
H1	0.739 (5)	0.423 (3)	0.1724 (11)	0.082 (11)*	

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0515 (11)	0.0691 (13)	0.0553 (11)	−0.0176 (10)	0.0101 (9)	−0.0149 (10)
O2	0.0232 (10)	0.141 (2)	0.0983 (18)	−0.0018 (12)	0.0063 (10)	−0.0682 (17)
O3	0.0291 (10)	0.131 (2)	0.0915 (16)	0.0101 (11)	0.0009 (10)	−0.0680 (16)
O4	0.0235 (9)	0.152 (2)	0.0618 (12)	0.0044 (12)	0.0002 (8)	−0.0417 (14)
O5	0.0306 (9)	0.0669 (11)	0.0482 (10)	0.0073 (9)	0.0045 (8)	−0.0080 (9)
N1	0.0605 (16)	0.0487 (13)	0.0666 (16)	−0.0138 (12)	−0.0207 (13)	0.0029 (12)
N2	0.0406 (11)	0.0381 (10)	0.0430 (10)	0.0058 (9)	0.0081 (9)	−0.0021 (9)
C1	0.0628 (18)	0.0453 (14)	0.0510 (15)	−0.0064 (14)	−0.0091 (14)	0.0023 (11)
C2	0.0486 (16)	0.0426 (14)	0.0641 (17)	−0.0055 (12)	−0.0159 (13)	0.0105 (13)
C3	0.0415 (17)	0.0646 (19)	0.096 (3)	−0.0155 (15)	−0.0073 (16)	0.0174 (19)
C4	0.054 (2)	0.077 (2)	0.098 (3)	−0.0126 (17)	0.0181 (18)	0.006 (2)
C5	0.060 (2)	0.073 (2)	0.073 (2)	−0.0121 (16)	0.0139 (16)	−0.0047 (17)
C6	0.0463 (16)	0.0497 (15)	0.0580 (16)	−0.0083 (12)	−0.0004 (12)	0.0037 (13)
C7	0.0413 (14)	0.0375 (13)	0.0517 (14)	−0.0033 (10)	−0.0075 (11)	0.0075 (11)
C8	0.0467 (14)	0.0356 (12)	0.0498 (13)	−0.0013 (11)	−0.0074 (11)	0.0039 (10)
C9	0.0431 (14)	0.0412 (13)	0.0478 (13)	0.0012 (11)	−0.0017 (11)	−0.0015 (11)
C10	0.0356 (13)	0.0432 (12)	0.0447 (12)	0.0030 (11)	0.0053 (10)	−0.0013 (11)
C11	0.048 (5)	0.049 (4)	0.058 (5)	−0.003 (3)	0.002 (4)	0.019 (4)

C12	0.129 (10)	0.059 (6)	0.114 (9)	0.032 (7)	0.013 (7)	0.012 (5)
C13	0.115 (9)	0.098 (10)	0.062 (6)	0.019 (8)	−0.018 (5)	0.033 (5)
C11A	0.045 (5)	0.053 (4)	0.064 (5)	−0.001 (3)	0.002 (4)	0.010 (3)
C12A	0.126 (10)	0.044 (5)	0.117 (8)	0.028 (6)	0.018 (7)	0.006 (5)
C13A	0.111 (8)	0.072 (7)	0.091 (8)	−0.002 (6)	−0.025 (7)	0.025 (6)
C14	0.0531 (16)	0.0514 (14)	0.0490 (14)	−0.0098 (13)	−0.0036 (12)	−0.0052 (12)
C15	0.087 (3)	0.107 (3)	0.063 (2)	−0.029 (2)	0.0059 (18)	−0.033 (2)
C16	0.0541 (17)	0.077 (2)	0.074 (2)	−0.0149 (17)	−0.0052 (16)	0.0004 (17)
C17	0.0242 (12)	0.0787 (19)	0.0558 (15)	0.0062 (13)	0.0005 (11)	−0.0235 (15)
C18	0.0270 (12)	0.0701 (18)	0.0550 (14)	0.0015 (12)	0.0032 (11)	−0.0246 (14)
C19	0.0284 (12)	0.0645 (17)	0.0434 (12)	0.0076 (12)	0.0016 (10)	−0.0127 (12)
C20	0.0258 (11)	0.0672 (16)	0.0382 (12)	0.0038 (11)	0.0038 (10)	−0.0017 (12)

Geometric parameters (Å, °)

O1—C6	1.365 (3)	C11—H11	0.9800
O1—H1	0.891 (13)	C11—C12	1.512 (9)
O2—H2A	0.908 (14)	C11—C13	1.512 (9)
O2—C17	1.260 (3)	C12—H12A	0.9600
O3—C17	1.206 (3)	C12—H12B	0.9600
O4—C20	1.260 (3)	C12—H12C	0.9600
O5—C20	1.235 (3)	C13—H13A	0.9600
N1—C1	1.366 (4)	C13—H13B	0.9600
N1—C2	1.359 (4)	C13—H13C	0.9600
N1—H1A	0.870 (13)	C11A—H11A	0.9800
N2—C10	1.504 (3)	C11A—C12A	1.494 (9)
N2—C11	1.543 (9)	C11A—C13A	1.506 (9)
N2—C11A	1.515 (10)	C12A—H12D	0.9600
N2—C14	1.536 (3)	C12A—H12E	0.9600
N2—H2	0.899 (13)	C12A—H12F	0.9600
C1—H1B	0.9300	C13A—H13D	0.9600
C1—C8	1.363 (4)	C13A—H13E	0.9600
C2—C3	1.400 (4)	C13A—H13F	0.9600
C2—C7	1.409 (4)	C14—H14	0.9800
C3—H3	0.9300	C14—C15	1.517 (4)
C3—C4	1.357 (5)	C14—C16	1.515 (4)
C4—H4	0.9300	C15—H15A	0.9600
C4—C5	1.402 (5)	C15—H15B	0.9600
C5—H5	0.9300	C15—H15C	0.9600
C5—C6	1.366 (4)	C16—H16A	0.9600
C6—C7	1.411 (4)	C16—H16B	0.9600
C7—C8	1.437 (4)	C16—H16C	0.9600
C8—C9	1.503 (4)	C17—C18	1.488 (3)
C9—H9A	0.9700	C18—H18	0.9300
C9—H9B	0.9700	C18—C19	1.290 (3)
C9—C10	1.516 (4)	C19—H19	0.9300
C10—H10A	0.9700	C19—C20	1.493 (3)
C10—H10B	0.9700		

C6—O1—H1	108 (2)	C11—C12—H12C	109.5
C17—O2—H2A	116 (4)	H12A—C12—H12B	109.5
C1—N1—H1A	126 (3)	H12A—C12—H12C	109.5
C2—N1—C1	109.2 (2)	H12B—C12—H12C	109.5
C2—N1—H1A	125 (3)	C11—C13—H13A	109.5
C10—N2—C11	109.8 (7)	C11—C13—H13B	109.5
C10—N2—C11A	117.0 (6)	C11—C13—H13C	109.5
C10—N2—C14	112.97 (18)	H13A—C13—H13B	109.5
C10—N2—H2	105.3 (16)	H13A—C13—H13C	109.5
C11—N2—H2	100.3 (17)	H13B—C13—H13C	109.5
C11A—N2—C14	108.7 (8)	N2—C11A—H11A	107.0
C11A—N2—H2	108.2 (17)	C12A—C11A—N2	116.2 (10)
C14—N2—C11	122.2 (8)	C12A—C11A—H11A	107.0
C14—N2—H2	103.7 (16)	C12A—C11A—C13A	112.5 (11)
N1—C1—H1B	124.8	C13A—C11A—N2	106.7 (11)
C8—C1—N1	110.4 (3)	C13A—C11A—H11A	107.0
C8—C1—H1B	124.8	C11A—C12A—H12D	109.5
N1—C2—C3	129.7 (3)	C11A—C12A—H12E	109.5
N1—C2—C7	107.5 (3)	C11A—C12A—H12F	109.5
C3—C2—C7	122.8 (3)	H12D—C12A—H12E	109.5
C2—C3—H3	121.7	H12D—C12A—H12F	109.5
C4—C3—C2	116.6 (3)	H12E—C12A—H12F	109.5
C4—C3—H3	121.7	C11A—C13A—H13D	109.5
C3—C4—H4	118.8	C11A—C13A—H13E	109.5
C3—C4—C5	122.5 (3)	C11A—C13A—H13F	109.5
C5—C4—H4	118.8	H13D—C13A—H13E	109.5
C4—C5—H5	119.5	H13D—C13A—H13F	109.5
C6—C5—C4	121.0 (3)	H13E—C13A—H13F	109.5
C6—C5—H5	119.5	N2—C14—H14	106.2
O1—C6—C5	123.8 (3)	C15—C14—N2	113.9 (3)
O1—C6—C7	117.2 (2)	C15—C14—H14	106.2
C5—C6—C7	118.9 (3)	C16—C14—N2	111.5 (2)
C2—C7—C6	118.2 (2)	C16—C14—H14	106.2
C2—C7—C8	107.1 (2)	C16—C14—C15	112.3 (3)
C6—C7—C8	134.8 (2)	C14—C15—H15A	109.5
C1—C8—C7	105.8 (2)	C14—C15—H15B	109.5
C1—C8—C9	125.6 (3)	C14—C15—H15C	109.5
C7—C8—C9	128.6 (2)	H15A—C15—H15B	109.5
C8—C9—H9A	109.5	H15A—C15—H15C	109.5
C8—C9—H9B	109.5	H15B—C15—H15C	109.5
C8—C9—C10	110.8 (2)	C14—C16—H16A	109.5
H9A—C9—H9B	108.1	C14—C16—H16B	109.5
C10—C9—H9A	109.5	C14—C16—H16C	109.5
C10—C9—H9B	109.5	H16A—C16—H16B	109.5
N2—C10—C9	113.63 (19)	H16A—C16—H16C	109.5
N2—C10—H10A	108.8	H16B—C16—H16C	109.5
N2—C10—H10B	108.8	O2—C17—C18	114.0 (2)

C9—C10—H10A	108.8	O3—C17—O2	125.1 (2)
C9—C10—H10B	108.8	O3—C17—C18	120.9 (2)
H10A—C10—H10B	107.7	C17—C18—H18	118.5
N2—C11—H11	107.4	C19—C18—C17	123.0 (2)
C12—C11—N2	112.5 (9)	C19—C18—H18	118.5
C12—C11—H11	107.4	C18—C19—H19	117.8
C13—C11—N2	111.5 (10)	C18—C19—C20	124.3 (2)
C13—C11—H11	107.4	C20—C19—H19	117.8
C13—C11—C12	110.2 (11)	O4—C20—C19	114.1 (2)
C11—C12—H12A	109.5	O5—C20—O4	125.2 (2)
C11—C12—H12B	109.5	O5—C20—C19	120.8 (2)
O1—C6—C7—C2	179.3 (2)	C6—C7—C8—C9	0.2 (5)
O1—C6—C7—C8	−1.4 (4)	C7—C2—C3—C4	0.2 (4)
O2—C17—C18—C19	173.0 (3)	C7—C8—C9—C10	75.9 (3)
O3—C17—C18—C19	−7.1 (5)	C8—C9—C10—N2	170.4 (2)
N1—C1—C8—C7	−0.3 (3)	C10—N2—C11—C12	−52.0 (12)
N1—C1—C8—C9	−179.5 (2)	C10—N2—C11—C13	72.4 (13)
N1—C2—C3—C4	−179.3 (3)	C10—N2—C11A—C12A	−57.9 (12)
N1—C2—C7—C6	179.2 (2)	C10—N2—C11A—C13A	68.4 (13)
N1—C2—C7—C8	−0.3 (3)	C10—N2—C14—C15	54.5 (3)
C1—N1—C2—C3	179.6 (3)	C10—N2—C14—C16	−177.2 (2)
C1—N1—C2—C7	0.1 (3)	C11—N2—C10—C9	−164.4 (7)
C1—C8—C9—C10	−105.0 (3)	C11—N2—C14—C15	−80.1 (6)
C2—N1—C1—C8	0.1 (3)	C11—N2—C14—C16	48.1 (6)
C2—C3—C4—C5	0.3 (5)	C11A—N2—C10—C9	−177.3 (8)
C2—C7—C8—C1	0.3 (3)	C11A—N2—C14—C15	−77.0 (6)
C2—C7—C8—C9	179.6 (2)	C11A—N2—C14—C16	51.2 (6)
C3—C2—C7—C6	−0.3 (4)	C14—N2—C10—C9	55.3 (3)
C3—C2—C7—C8	−179.8 (3)	C14—N2—C11—C12	83.9 (12)
C3—C4—C5—C6	−0.6 (6)	C14—N2—C11—C13	−151.7 (11)
C4—C5—C6—O1	−178.8 (3)	C14—N2—C11A—C12A	71.5 (13)
C4—C5—C6—C7	0.5 (5)	C14—N2—C11A—C13A	−162.2 (12)
C5—C6—C7—C2	0.0 (4)	C17—C18—C19—C20	−177.7 (3)
C5—C6—C7—C8	179.3 (3)	C18—C19—C20—O4	174.1 (3)
C6—C7—C8—C1	−179.1 (3)	C18—C19—C20—O5	−6.3 (4)

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O2—H2A $\cdots$ O4 ⁱ	0.91 (1)	1.54 (2)	2.441 (3)	173 (6)
N1—H1A $\cdots$ O5 ⁱⁱ	0.87 (1)	2.13 (2)	2.989 (3)	170 (4)
N2—H2 $\cdots$ O3	0.90 (1)	1.88 (1)	2.756 (3)	165 (2)
O1—H1 $\cdots$ O5 ⁱⁱⁱ	0.89 (1)	1.89 (1)	2.784 (3)	177 (4)

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