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N,*N*-Diethyl-4-glutaratotryptamine

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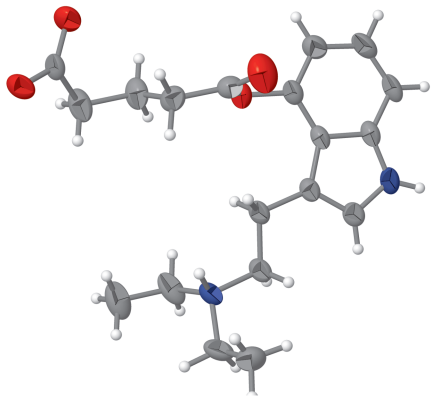
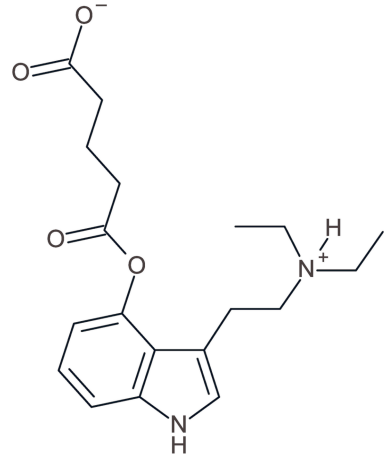
Structural data: full structural data are available from iucrdata.iucr.org

The synthesis and structure of the title compound, $C_{19}H_{26}N_2O_4$ [systematic name: 5-({3-[2-(diethylazaniumyl)ethyl]-1*H*-indol-4-yl}oxy)-5-oxopentanoate], are reported. The title compound exists as a zwitterion in the solid state with a protonated tertiary ammonium group and a deprotonated glutarato carboxylate group. In the extended structure, the tryptamine zwitterions dimerize through pairwise N—H···O hydrogen bonds, and additional N—H···O hydrogen bonds join these dimers together in an infinite two-dimensional network lying parallel to the $(10\bar{2})$ plane.

3D view



Chemical scheme



Structure description

Serotonergic pharmacology and potential therapeutic applications have stimulated renewed interest in 4-hydroxytryptamines and their prodrugs, most notably the natural products psilocin (4-hydroxy-*N*,*N*-dimethyltryptamine) and psilocybin (4-phosphoryloxy-*N*,*N*-dimethyltryptamine). Esterification of the 4-hydroxy group provides a route to synthetic prodrugs that release their active metabolite following hydrolysis, as demonstrated by the conversion of psilacetin (4-acetoxy-*N*,*N*-dimethyltryptamine) to psilocin *in vivo* (Jones *et al.*, 2024; Pego *et al.*, 2025). Other psilocin esters have been examined for the varied chemical stability and metabolic properties (Eklund *et al.*, 2025). The 4-glutarato substituent is of particular interest because it combines a cleavable ester linkage with a terminal carboxylic acid group. Together with the basic tertiary amine, this functionality permits zwitterion formation and introduces additional hydrogen bonding interactions. These features raise questions concerning protonation state, crystal packing and solvation, and their impact on aqueous solubility, dissolution and chemical stability. Consequently, characterization of the molecular structure and crystalline form is important for establishing the composition and molecular formula of the isolated material and for calculating molar concentrations in subsequent physicochemical and biological investigations.

We have previously reported the solid-state structures of more than a dozen ester prodrugs of 4-hydroxytryptamines (see below). Our investigations of 4-glutarato-*N*,*N*-

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diisopropyltryptamine provided the first crystal structures of this compound, identifying its methanol and ethanol monosolvates (Naeem, Bauer *et al.*, 2022). Both structures established a zwitterionic molecule, with a protonated amine and deprotonated terminal carboxylate group, and demonstrated stoichiometric incorporation of alcohol within the extended structure. Subsequent single-crystal characterization identified a 2-propanol monosolvate (Bryson & Nap, 2026), showing that there are multiple distinct solvent-containing crystalline forms of this prodrug.

The pharmacological relevance of the 4-glutarato group is illustrated by Reunion Neuroscience's clinical drug candidate, RE104, a prodrug of 4-hydroxy-*N*,*N*-diisopropyltryptamine. Conversion to the parent hydroxy compound was demonstrated in preclinical investigations (Bryson *et al.*, 2024), followed by clinical investigation of its pharmacokinetics and psychoactive effects in healthy volunteers (Ludbrook *et al.*, 2025). The preclinical report also describes solvent retention during preparation and uses both hydrochloride and zwitterionic terminology for the material. These observations highlight the importance of establishing the chemical form and solvent content of the isolated solid. We previously noted that solvate formation could contribute to the reported purification difficulties (Naeem *et al.*, 2025), although residual solvent alone does not establish crystalline solvate. Determining protonation state, counter-ion content and solvation is therefore important when assigning molecular formulae and interpreting concentration-dependent biological measurements.

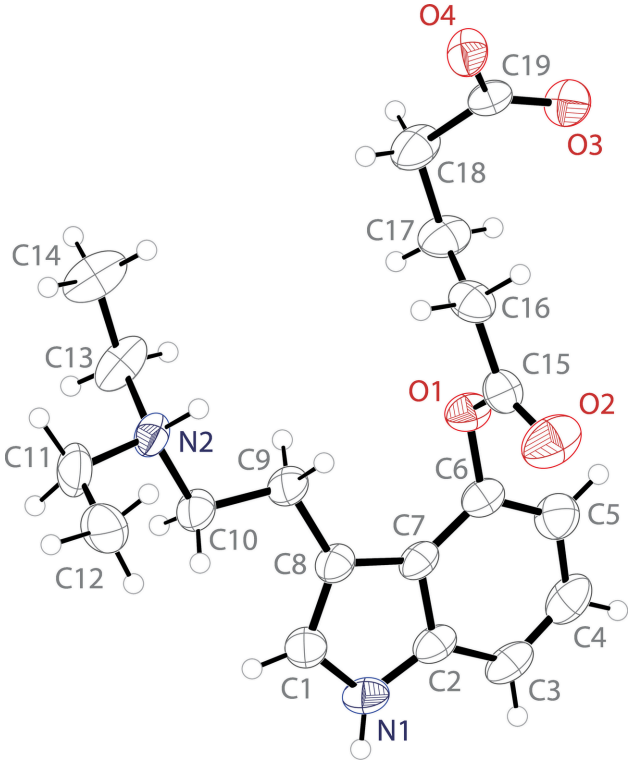

Figure 1
The molecular structure of (**I**) showing displacement ellipsoids drawn at the 50% probability level.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4^{i}	0.98 (1)	1.66 (1)	2.6363 (16)	178 (2)
N1—H1···O3^{ii}	0.86 (1)	1.99 (1)	2.8182 (16)	161 (2)

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

Recently, we reported the crystal structures of 4-hydroxy-*N*,*N*-diethylammonium hydrofumarate and the corresponding 4-acetoxy prodrug as its fumarate-fumaric acid salt/adduct (Naeem *et al.*, 2026). Herein, we extend these investigations to *N*,*N*-diethyl-4-glutaratotryptamine, $C_{19}H_{26}N_2O_4$ (**I**), a putative prodrug of 4-hydroxy-*N*,*N*-diethyltryptamine. The title compound crystallizes as an unsolvated zwitterion, allowing for comparison with the alcohol-solvated *N*,*N*-diisopropyl analogue.

Compound (**I**) exists in the solid-state as a zwitterion, with a protonated tertiary ammonium group and a deprotonated carboxylate anion on the glutarato group. The asymmetric unit contains a single zwitterionic molecule (Fig. 1). The C1–C8/N1 indole unit is near planar with an r.m.s. deviation from planarity of 0.012 Å. The glutarato unit is turned nearly perpendicular to the indole plane demonstrated by a C7—C6—O1—C15 torsion angle of 95.37 (16)°. By contrast, the ethylamino arm is almost in plane with the indole ring system as demonstrated by a C7—C8—C9—C10 torsion angle of 177.58 (13)°. The ethylamino arm demonstrates an *anti* conformation with a C8—C9—C10—N2 torsion angle of 172.46 (10)°.

In the extended structure of (**I**), there are pairwise N2—H2···O4 bonds (Table 1) between the diethyltryptammonium cation and the carboxylate anion of another zwitterionic molecule. These interactions form centrosymmetric dimers (Fig. 2), which form rings with graph-set notation of $R_2^2(28)$ (Etter *et al.*, 1990). The dimers are joined together through N1—H1···O3 hydrogen bonds between the indole nitrogen atom and a carboxylate oxygen atom of another molecule. These interactions combine to form a two-

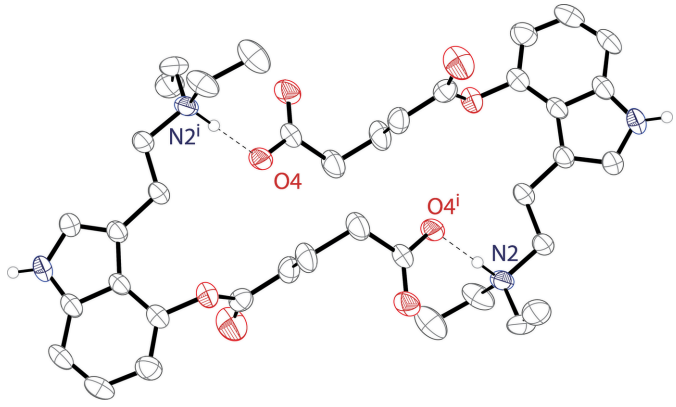

Figure 2
The ring formed by the dimerization of two zwitterionic molecules of (**I**) with graph set notation $R_2^2(28)$. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding are omitted for clarity. Symmetry code: (i) $2-x, 1-y, 1-z$.

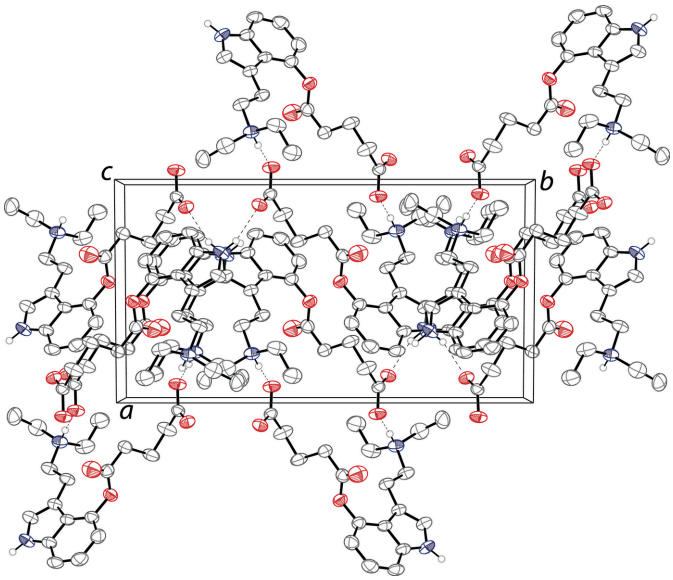

Figure 3
The packing of (**I**) viewed along the *c*-axis direction. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding are omitted for clarity.

dimensional network lying in the (10$\bar{2}$) plane. The packing diagram of (**I**) is shown in Fig. 3.

The literature structures most closely related to (**I**) are the ethanol and methanol solvates of 4-glutarato-*N*,*N*-diisopropyltryptamine (Naeem, Bauer *et al.*, 2022; Cambridge Structural Database refcodes TEKWOZ, TEKWUF). There are three structures reported in the literature that posses *N*,*N*-diethyltryptamine cores, which are 4-phosphoryloxy-*N*,*N*-diethyltryptamine (Baker *et al.*, 1973; KOWHOT) as well as 4-hydroxy-*N*,*N*-diethyltrpytamine as its hydrofumarate salt and 4-acetoxy-*N*,*N*-diethyltryptamine as its fumarate salt with a fumaric acid adduct (Naeem *et al.*, 2026). Beyond the structures of 4-glutarato-*N*,*N*-diisopropyltryptamine, there are eleven structures of 4-substituted esters of tryptamines. Ten of these esters are 4-acetoxy derivatives that include psilacetin, 4-acetoxy-*N*,*N*-dimethyltryptamine, as its hydrofumarate (Chadeayne *et al.*, 2019*a*: HOCJUH) and fumarate (Chadeayne *et al.*, 2019*b*: XOFDOO) salts, 4-acetoxy-*N*-methyl-*N*-ethyltryptamine as its hydrofumarate salt, 4-acetoxy-*N*-methyl-*N*-allyltryptamine as its hydrofumarate salt, 4-acetoxy-*N*,*N*-diallyltryptamine as its fumarate/fumaric acid (Pham *et al.*, 2021: OJIQIK, OJIQOQ, OJIQUW), 4-acetoxy-*N*,*N*,*N*-timethyltryptammonium iodide (Chadeayne, Pham, Reid *et al.*, 2020: XUXDUS), 4-acetoxy-*N*-ethyl-*N*,*N*-dimethyltryptammonium iodide, 4-acetoxy-*N*-propyl-*N*,*N*-dimethyltryptammonium iodide, 4-acetoxy-*N*-isopropyl-*N*,*N*-dimethyltryptammonium iodide (Glatfelter, Pham *et al.*, 2022: EDOZEG, EDOYOP, EDZAC), and 4-acetoxy-*N*-methyltryptamine as its chloride salt (Glatfelter, Pottie *et al.*, 2022). There is also one reported 4-propionoxy tryptamine ester, which is the hydrofumarate salt of 4-propionoxy-*N*,*N*-dimethyltryptamine (Glatfelter *et al.*, 2023). There are five zwitterionic tryptamine structures reported, which are the two aforementioned 4-glutarato-*N*,*N*-diisopropyltryptamine structures, the aforementioned 4-phosphoryloxy-*N*,*N*-diethyltryptamine structure, and two natural products, which are baeocystin, 4-phosphoryloxy-*N*-methyltryptamine (Naeem, Chadeayne *et al.*, 2022; FEJBAB) and psilocybin, 4-phosphoryloxy-*N*,*N*-dimethyltryptamine (Weber & Petcher, 1974; PSILOC; Sherwood *et al.*, 2022; TAVZID, TAVZID01).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{26}N_2O_4$
M_r	346.42
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	300
a, b, c (Å)	10.2324 (5), 18.8638 (11), 9.7347 (5)
β (°)	100.419 (2)
V (Å^3)	1848.03 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.35 × 0.30 × 0.25
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.589, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	49940, 3790, 3199
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.128, 1.06
No. of reflections	3790
No. of parameters	236
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.22

Computer programs: *APEX4* and *SAINT* (Bruker, 2021), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

70 mg (1.0 mmol) of 4-hydroxy-*N*,*N*-diethyltryptamine were dissolved in 5 ml of chloroform and 0.20 ml of triethylamine. 343 mg (10.0 mmol) of glutaric anhydride was added to the mixture and it was stirred at room temperature for 12 h. The resulting precipitate was isolated *via* filtration and washed with chloroform (5 ml) to yield the title compound as a white powder (35 mg, 50% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.04 (*br s*, 1H, N*H*), 8.31 (*s*, 1H, N*H*), 7.22 (*d*, J = 8.1 Hz, 1H, Ar*H*), 7.15 (*d*, J = 2.3 Hz, 1H, Ar*H*), 7.03 (*t*, J = 7.9 Hz, 1H, Ar*H*), 6.65 (*d*, J = 7.6 Hz, 1H, Ar*H*), 2.85–2.67 (*m*, 6H, CH_2), 2.63 (*q*, J = 7.1 Hz, 4H, CH_2), 2.30 (*t*, J = 7.1 Hz, 2H, CH_2), 1.87 (*p*, J = 7.2 Hz, 2H, CH_2), 1.01 (*t*, J = 7.1 Hz, 6H, CH_3).

The product was recrystallized by being dissolved in a boiling methanol/ethyl acetate solution and cooled to yield colourless blocks of (**I**) suitable for X-ray analysis.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2026). **11**, x261184 [https://doi.org/10.1107/S2414314626011843]

N,*N*-Diethyl-4-glutaratotryptamine

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5-({3-[2-(Diethylazaniumyl)ethyl]-1*H*-indol-4-yl}oxy)-5-oxopentanoate

Crystal data

$C_{19}H_{26}N_2O_4$
M_r = 346.42
Monoclinic, $P2_1/c$
a = 10.2324 (5) Å
b = 18.8638 (11) Å
c = 9.7347 (5) Å
β = 100.419 (2)°
V = 1848.03 (17) Å^3
Z = 4
$F(000)$ = 744
D_x = 1.245 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9975 reflections
θ = 2.9–26.3°
μ = 0.09 mm^{-1}
T = 300 K
Block, colourless
0.35 × 0.30 × 0.25 mm

Data collection

Bruker D8 Venture CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.589, T_{max} = 0.745
49940 measured reflections
3790 independent reflections
3199 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 26.4°, θ_{min} = 3.0°
h = −12→11
k = −23→23
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.128
S = 1.06
3790 reflections
236 parameters
2 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.5947P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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 and H2 were found in a difference-Fourier map and were refined isotropically, using *DFIX* restraints with the N—H(indole) distance set at 0.87 (1) Å and the N—H(ammonium) distance set at 0.98 (1) Å. Isotropic displacement parameters were set to 1.2U_{eq} of the parent nitrogen atoms. All other H atoms were placed in calculated positions and refined as riding atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.54565 (10)	0.46267 (6)	0.28973 (11)	0.0425 (3)
O2	0.67174 (14)	0.41993 (8)	0.14419 (15)	0.0711 (4)
O3	0.89104 (10)	0.65738 (6)	0.27311 (12)	0.0487 (3)
O4	1.06473 (10)	0.63014 (6)	0.43491 (11)	0.0467 (3)
N1	0.32512 (13)	0.24916 (8)	0.31528 (15)	0.0474 (3)
N2	0.78065 (12)	0.32285 (7)	0.73441 (12)	0.0391 (3)
C1	0.42928 (15)	0.25527 (9)	0.42540 (16)	0.0444 (4)
H1A	0.452589	0.221239	0.494633	0.053*
C2	0.31990 (14)	0.30866 (8)	0.23515 (15)	0.0388 (3)
C3	0.23244 (15)	0.32722 (9)	0.11282 (16)	0.0463 (4)
H3	0.162317	0.297727	0.074895	0.056*
C4	0.25361 (17)	0.39032 (10)	0.05078 (18)	0.0531 (4)
H4	0.197029	0.403546	−0.031035	0.064*
C5	0.35857 (17)	0.43558 (9)	0.10752 (18)	0.0495 (4)
H5	0.371448	0.477994	0.063105	0.059*
C6	0.44183 (14)	0.41694 (8)	0.22856 (15)	0.0391 (3)
C7	0.42580 (13)	0.35336 (8)	0.29642 (14)	0.0348 (3)
C8	0.49397 (13)	0.31825 (8)	0.41924 (14)	0.0366 (3)
C9	0.60952 (14)	0.34755 (9)	0.52114 (15)	0.0406 (3)
H9A	0.584227	0.392693	0.556232	0.049*
H9B	0.683064	0.356003	0.472827	0.049*
C10	0.65480 (14)	0.29825 (9)	0.64301 (15)	0.0429 (4)
H10A	0.585334	0.294801	0.698560	0.052*
H10B	0.668764	0.251298	0.607674	0.052*
C11	0.84691 (19)	0.26272 (11)	0.82148 (17)	0.0570 (5)
H11A	0.918146	0.281640	0.891249	0.068*
H11B	0.782766	0.240746	0.870265	0.068*
C12	0.9028 (2)	0.20718 (10)	0.7387 (2)	0.0632 (5)
H12A	0.950660	0.172798	0.801112	0.095*
H12B	0.961920	0.228930	0.685071	0.095*
H12C	0.831651	0.184177	0.676945	0.095*
C13	0.75497 (17)	0.38435 (12)	0.82325 (19)	0.0594 (5)
H13A	0.707550	0.367547	0.894638	0.071*
H13B	0.698133	0.418093	0.765534	0.071*
C14	0.8793 (2)	0.42165 (13)	0.8927 (2)	0.0722 (6)
H14A	0.856586	0.458547	0.952097	0.108*
H14B	0.923058	0.441941	0.822690	0.108*
H14C	0.937544	0.388298	0.947528	0.108*
C15	0.66096 (15)	0.45670 (8)	0.24087 (16)	0.0405 (3)
C16	0.77034 (15)	0.49948 (8)	0.32583 (18)	0.0452 (4)
H16A	0.828576	0.515787	0.264053	0.054*
H16B	0.822016	0.468188	0.393934	0.054*
C17	0.72981 (15)	0.56314 (10)	0.40273 (19)	0.0518 (4)
H17A	0.674152	0.547736	0.467825	0.062*
H17B	0.678134	0.595266	0.336330	0.062*

C18	0.85087 (17)	0.60217 (12)	0.48231 (18)	0.0573 (5)
H18A	0.820817	0.640577	0.535115	0.069*
H18B	0.901990	0.569724	0.548439	0.069*
C19	0.94092 (13)	0.63241 (8)	0.38828 (15)	0.0367 (3)
H2	0.8387 (16)	0.3389 (10)	0.6714 (17)	0.058 (5)*
H1	0.2714 (17)	0.2136 (8)	0.299 (2)	0.065 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0360 (5)	0.0443 (6)	0.0467 (6)	−0.0065 (4)	0.0059 (4)	−0.0071 (5)
O2	0.0602 (8)	0.0872 (10)	0.0700 (9)	−0.0054 (7)	0.0225 (7)	−0.0285 (8)
O3	0.0354 (6)	0.0513 (7)	0.0541 (7)	0.0067 (5)	−0.0066 (5)	0.0048 (5)
O4	0.0281 (5)	0.0680 (7)	0.0411 (6)	−0.0042 (5)	−0.0011 (4)	0.0096 (5)
N1	0.0378 (7)	0.0529 (8)	0.0489 (8)	−0.0187 (6)	0.0009 (6)	−0.0045 (6)
N2	0.0335 (6)	0.0551 (8)	0.0271 (6)	−0.0025 (5)	0.0013 (5)	−0.0006 (5)
C1	0.0364 (8)	0.0536 (9)	0.0417 (8)	−0.0113 (6)	0.0029 (6)	0.0020 (7)
C2	0.0284 (7)	0.0490 (8)	0.0381 (7)	−0.0051 (6)	0.0034 (6)	−0.0105 (6)
C3	0.0297 (7)	0.0611 (10)	0.0437 (8)	−0.0040 (7)	−0.0049 (6)	−0.0146 (7)
C4	0.0425 (9)	0.0652 (11)	0.0443 (9)	0.0086 (8)	−0.0117 (7)	−0.0058 (8)
C5	0.0475 (9)	0.0485 (9)	0.0482 (9)	0.0046 (7)	−0.0027 (7)	0.0019 (7)
C6	0.0329 (7)	0.0433 (8)	0.0393 (7)	−0.0020 (6)	0.0019 (6)	−0.0069 (6)
C7	0.0254 (6)	0.0462 (8)	0.0315 (7)	−0.0031 (5)	0.0021 (5)	−0.0079 (6)
C8	0.0279 (7)	0.0467 (8)	0.0345 (7)	−0.0053 (6)	0.0038 (5)	−0.0034 (6)
C9	0.0307 (7)	0.0504 (9)	0.0378 (7)	−0.0078 (6)	−0.0017 (6)	−0.0002 (6)
C10	0.0340 (7)	0.0592 (10)	0.0341 (7)	−0.0115 (7)	0.0024 (6)	0.0018 (7)
C11	0.0593 (10)	0.0740 (12)	0.0336 (8)	−0.0035 (9)	−0.0023 (7)	0.0155 (8)
C12	0.0714 (12)	0.0482 (10)	0.0630 (11)	0.0031 (9)	−0.0069 (9)	0.0146 (9)
C13	0.0429 (9)	0.0874 (14)	0.0456 (9)	0.0082 (9)	0.0019 (7)	−0.0237 (9)
C14	0.0544 (11)	0.0836 (15)	0.0748 (13)	0.0018 (10)	0.0013 (10)	−0.0361 (11)
C15	0.0410 (8)	0.0400 (8)	0.0412 (8)	0.0038 (6)	0.0088 (6)	0.0054 (6)
C16	0.0346 (8)	0.0440 (8)	0.0566 (9)	−0.0038 (6)	0.0073 (7)	0.0058 (7)
C17	0.0333 (8)	0.0634 (11)	0.0602 (10)	−0.0133 (7)	0.0125 (7)	−0.0126 (8)
C18	0.0420 (9)	0.0831 (13)	0.0487 (9)	−0.0215 (9)	0.0132 (7)	−0.0172 (9)
C19	0.0290 (7)	0.0383 (7)	0.0410 (8)	−0.0029 (5)	0.0014 (6)	−0.0090 (6)

Geometric parameters (Å, º)

O1—C6	1.4137 (17)	C9—H9B	0.9700
O1—C15	1.3543 (18)	C9—C10	1.513 (2)
O2—C15	1.190 (2)	C10—H10A	0.9700
O3—C19	1.2378 (18)	C10—H10B	0.9700
O4—C19	1.2668 (17)	C11—H11A	0.9700
N1—C1	1.373 (2)	C11—H11B	0.9700
N1—C2	1.362 (2)	C11—C12	1.497 (3)
N1—H1	0.864 (9)	C12—H12A	0.9600
N2—C10	1.5003 (18)	C12—H12B	0.9600
N2—C11	1.502 (2)	C12—H12C	0.9600

N2—C13	1.498 (2)	C13—H13A	0.9700
N2—H2	0.976 (9)	C13—H13B	0.9700
C1—H1A	0.9300	C13—C14	1.503 (3)
C1—C8	1.367 (2)	C14—H14A	0.9600
C2—C3	1.399 (2)	C14—H14B	0.9600
C2—C7	1.4167 (19)	C14—H14C	0.9600
C3—H3	0.9300	C15—C16	1.501 (2)
C3—C4	1.370 (3)	C16—H16A	0.9700
C4—H4	0.9300	C16—H16B	0.9700
C4—C5	1.405 (2)	C16—C17	1.512 (2)
C5—H5	0.9300	C17—H17A	0.9700
C5—C6	1.369 (2)	C17—H17B	0.9700
C6—C7	1.393 (2)	C17—C18	1.526 (2)
C7—C8	1.433 (2)	C18—H18A	0.9700
C8—C9	1.5044 (18)	C18—H18B	0.9700
C9—H9A	0.9700	C18—C19	1.522 (2)

C15—O1—C6	115.94 (11)	N2—C11—H11B	108.8
C1—N1—H1	126.0 (14)	H11A—C11—H11B	107.7
C2—N1—C1	108.82 (12)	C12—C11—N2	113.72 (13)
C2—N1—H1	125.2 (14)	C12—C11—H11A	108.8
C10—N2—C11	110.64 (13)	C12—C11—H11B	108.8
C10—N2—H2	106.2 (11)	C11—C12—H12A	109.5
C11—N2—H2	109.0 (11)	C11—C12—H12B	109.5
C13—N2—C10	111.13 (12)	C11—C12—H12C	109.5
C13—N2—C11	111.55 (13)	H12A—C12—H12B	109.5
C13—N2—H2	108.2 (11)	H12A—C12—H12C	109.5
N1—C1—H1A	124.7	H12B—C12—H12C	109.5
C8—C1—N1	110.63 (14)	N2—C13—H13A	108.9
C8—C1—H1A	124.7	N2—C13—H13B	108.9
N1—C2—C3	130.29 (14)	N2—C13—C14	113.55 (14)
N1—C2—C7	107.54 (13)	H13A—C13—H13B	107.7
C3—C2—C7	122.17 (15)	C14—C13—H13A	108.9
C2—C3—H3	121.1	C14—C13—H13B	108.9
C4—C3—C2	117.72 (14)	C13—C14—H14A	109.5
C4—C3—H3	121.1	C13—C14—H14B	109.5
C3—C4—H4	119.1	C13—C14—H14C	109.5
C3—C4—C5	121.70 (15)	H14A—C14—H14B	109.5
C5—C4—H4	119.1	H14A—C14—H14C	109.5
C4—C5—H5	120.2	H14B—C14—H14C	109.5
C6—C5—C4	119.66 (16)	O1—C15—C16	111.84 (13)
C6—C5—H5	120.2	O2—C15—O1	122.50 (15)
C5—C6—O1	120.60 (14)	O2—C15—C16	125.63 (15)
C5—C6—C7	121.39 (14)	C15—C16—H16A	108.0
C7—C6—O1	118.00 (12)	C15—C16—H16B	108.0
C2—C7—C8	107.22 (13)	C15—C16—C17	117.11 (13)
C6—C7—C2	117.35 (13)	H16A—C16—H16B	107.3
C6—C7—C8	135.42 (13)	C17—C16—H16A	108.0

C1—C8—C7	105.78 (12)	C17—C16—H16B	108.0
C1—C8—C9	128.29 (14)	C16—C17—H17A	109.4
C7—C8—C9	125.90 (13)	C16—C17—H17B	109.4
C8—C9—H9A	109.1	C16—C17—C18	111.36 (14)
C8—C9—H9B	109.1	H17A—C17—H17B	108.0
C8—C9—C10	112.58 (12)	C18—C17—H17A	109.4
H9A—C9—H9B	107.8	C18—C17—H17B	109.4
C10—C9—H9A	109.1	C17—C18—H18A	108.9
C10—C9—H9B	109.1	C17—C18—H18B	108.9
N2—C10—C9	112.54 (12)	H18A—C18—H18B	107.7
N2—C10—H10A	109.1	C19—C18—C17	113.55 (14)
N2—C10—H10B	109.1	C19—C18—H18A	108.9
C9—C10—H10A	109.1	C19—C18—H18B	108.9
C9—C10—H10B	109.1	O3—C19—O4	124.01 (14)
H10A—C10—H10B	107.8	O3—C19—C18	119.46 (14)
N2—C11—H11A	108.8	O4—C19—C18	116.53 (14)

O1—C6—C7—C2	178.93 (12)	C5—C6—C7—C2	0.0 (2)
O1—C6—C7—C8	−2.3 (2)	C5—C6—C7—C8	178.83 (16)
O1—C15—C16—C17	−25.8 (2)	C6—O1—C15—O2	6.4 (2)
O2—C15—C16—C17	156.14 (17)	C6—O1—C15—C16	−171.75 (12)
N1—C1—C8—C7	−0.40 (18)	C6—C7—C8—C1	−178.04 (16)
N1—C1—C8—C9	177.45 (14)	C6—C7—C8—C9	4.0 (3)
N1—C2—C3—C4	−177.75 (16)	C7—C2—C3—C4	1.3 (2)
N1—C2—C7—C6	178.14 (13)	C7—C8—C9—C10	177.58 (13)
N1—C2—C7—C8	−0.97 (16)	C8—C9—C10—N2	172.46 (12)
C1—N1—C2—C3	179.89 (16)	C10—N2—C11—C12	69.00 (19)
C1—N1—C2—C7	0.74 (17)	C10—N2—C13—C14	−167.04 (17)
C1—C8—C9—C10	0.1 (2)	C11—N2—C10—C9	−160.46 (13)
C2—N1—C1—C8	−0.21 (19)	C11—N2—C13—C14	69.0 (2)
C2—C3—C4—C5	−0.5 (3)	C13—N2—C10—C9	75.05 (17)
C2—C7—C8—C1	0.83 (16)	C13—N2—C11—C12	−166.74 (16)
C2—C7—C8—C9	−177.08 (13)	C15—O1—C6—C5	−85.73 (18)
C3—C2—C7—C6	−1.1 (2)	C15—O1—C6—C7	95.37 (16)
C3—C2—C7—C8	179.79 (13)	C15—C16—C17—C18	−179.00 (14)
C3—C4—C5—C6	−0.5 (3)	C16—C17—C18—C19	62.4 (2)
C4—C5—C6—O1	−178.10 (14)	C17—C18—C19—O3	37.1 (2)
C4—C5—C6—C7	0.8 (2)	C17—C18—C19—O4	−142.92 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.98 (1)	1.66 (1)	2.6363 (16)	178 (2)
N1—H1···O3^{ii}	0.86 (1)	1.99 (1)	2.8182 (16)	161 (2)

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