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Bis(4-hydroxy-*N*,*N*-di-*n*-propyltryptammonium) fumarate tetrahydrate

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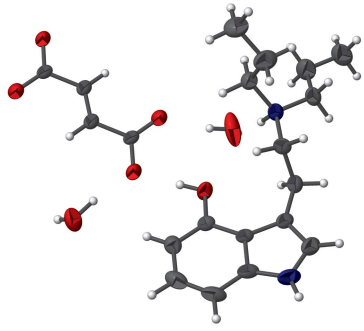
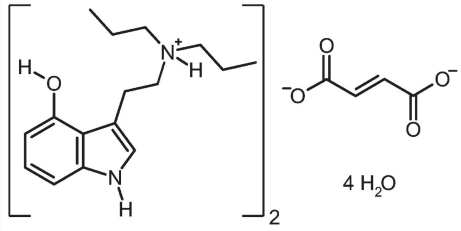
The title compound (systematic name: bis{[2-(4-hydroxy-1*H*-indol-3-yl)ethyl]bis(propan-2-yl)azanium} but-2-enedioate tetrahydrate), $2C_{16}H_{25}N_2O^+\cdot C_4H_2O_4^{2-}\cdot 4H_2O$, has a singly protonated DPT cation, one half of a fumarate dianion (completed by a crystallographic centre of symmetry) and two water molecules of crystallization in the asymmetric unit. A series of N—H···O and O—H···O hydrogen bonds form a three-dimensional network in the solid state.

3D view



Chemical scheme



Structure description

4-Hydroxy-*N*,*N*-di-*n*-propyltryptamine, or 4-HO-DPT, is a derivative of psilocin, which is the primary active psychedelic in 'magic' mushrooms. Psilocin is the metabolite of psilocybin and its synthetic analogue psilacetin, and is a serotonin-2a agonist which results in its mood-altering effects. Tryptamines, both naturally occurring [Psilocybin (Weber & Petcher, 1974), Psilocin (Petcher & Weber, 1974), and DMT (Falkenberg, 1972)] and their synthetic derivatives [Psilacetin (Chadeayne *et al.* 2019*a*,*b*), MPT (Chadeayne *et al.* 2019*c*), MiPT, and 4-HO-MiPT (Chadeayne, Pham *et al.* 2019)] have garnered a great deal of interest because of their potential to treat depression and post-traumatic stress disorder (PTSD) (Carhart-Harris & Goodwin, 2017). The solid-state structures of bioactive tryptamine molecules are significant because they define each molecule's physical identity, thereby providing the foundation for all downstream research. For example, such fundamental structural characterization is essential for understanding each molecule's biological and clinical properties *via* structure-activity relationships. To help further elucidate these properties, we report the structure of 4-HO-DPT herein.

The synthesis of 4-HO-DPT was first reported by Repke *et al.* in 1977 (Repke *et al.*, 1977). The molecular structure of bis(4-hydroxy-*N*,*N*-di-*n*-propyltryptammonium)-

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

Cg is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3^{i}	0.89 (3)	2.08 (3)	2.926 (2)	157 (2)
N2—H2···O1*W*	0.98 (2)	1.73 (3)	2.689 (2)	168 (2)
O1—H1···O2	0.88 (3)	1.74 (3)	2.625 (2)	174 (3)
O1*W*—H1*WA*···O2*W*^{ii}	0.83 (3)	1.88 (3)	2.710 (3)	172 (3)
O1*W*—H1*WB*···O3	0.83 (3)	1.86 (3)	2.684 (3)	171 (3)
O2*W*—H2*WB*···O2	0.94 (3)	1.76 (3)	2.695 (2)	173 (3)
O2*W*—H2*WA*···*Cg*^{iii}	0.82 (4)	2.69 (4)	3.488 (2)	167 (3)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x-1, y, z$; (iii) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

fumarate is shown in Fig. 1. The asymmetric unit contains one 4-HO-DPT cation, protonated at the dipropylamine N atom. There are also two independent water molecules, and half of a fumarate ion present. The 4-hydroxy-*N*,*N*-di-*n*-propyltryptammonium cations, fumarate dianions and water molecules are linked to each other in an infinite three-dimensional network through hydrogen bonds (Fig. 2, Table 1). Both inequivalent O atoms on the fumarate dianion (*i.e.* O2 and O3) accept two hydrogen bonds. One oxygen accepts hydrogen bonds from the hydroxide of the DPT cation and one water molecule. The other oxygen interacts with the indole N atom and the second independent water molecule. The ammonium proton hydrogen bonds with one of the water molecules. A weak O—H···π interaction is observed between one hydrogen atom of one of the water molecules and the six-membered ring of an adjacent indole unit. The packing of the compound is shown in Fig. 3.

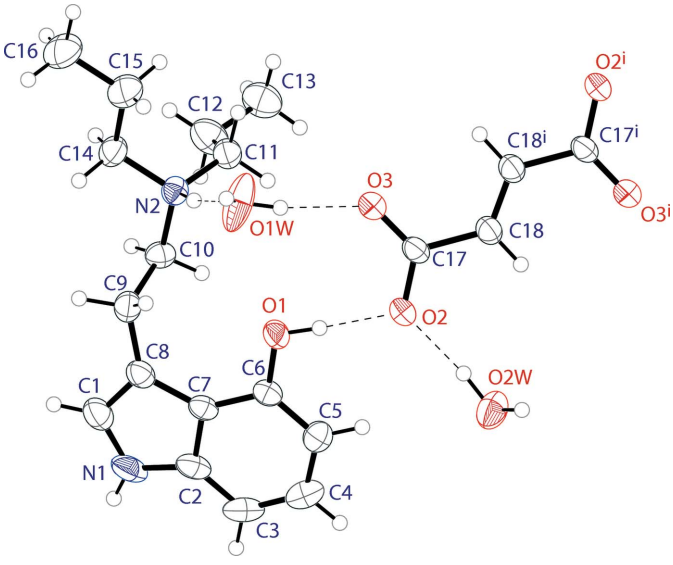


Figure 1
The molecular structure of bis(4-hydroxy-*N*,*N*-di-*n*-propyltryptammonium)fumarate tetrahydrate, showing the atomic labeling. Displacement ellipsoids are drawn at 50% probability level. Hydrogen bonds are shown as dashed lines. Symmetry code: (i) $2-x, 1-y, -z$.

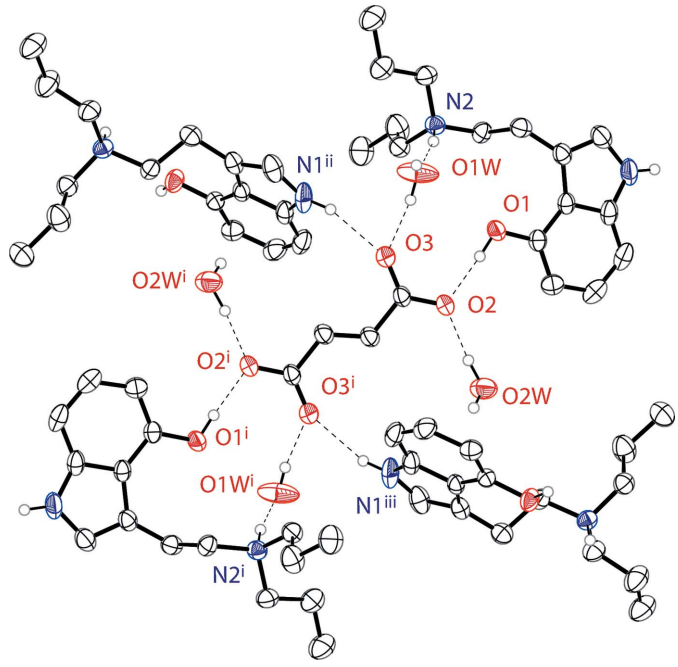


Figure 2
The hydrogen bonding of the fumarate ion in the structure of the title compound (Table 1), with hydrogen bonds shown as dashed lines. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms not involved in hydrogen bonds are omitted for clarity. Symmetry codes: (i) $2-x, 1-y, -z$; (ii) $-\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$; (iii) $\frac{5}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$.

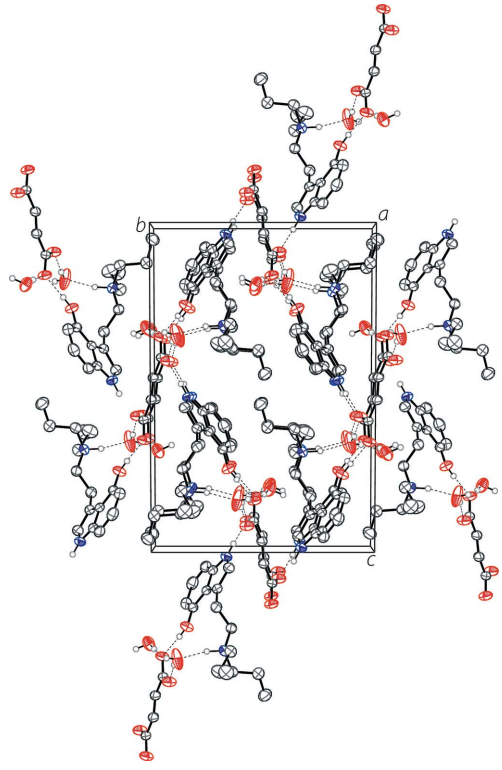


Figure 3
The crystal packing of the title compound, viewed along the *a* axis. The N—H···O and O—H···O hydrogen bonds (Table 1) are shown as dashed lines. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms not involved in hydrogen bonding are omitted for clarity.

Synthesis and crystallization

Single crystals of 4-HO-DPT fumarate suitable for X-ray analysis were obtained by the slow evaporation of an aqueous solution of a commercial sample of 4-hydroxy-*N*,*N*-di-*n*-propyltryptamine fumarate (The Indole Shop).

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{25}N_2O^+\cdot0.5C_4H_2O_4^{2-}\cdot2H_2O$
M_r	354.44
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	200
a, b, c (Å)	8.3495 (8), 12.5138 (11), 18.6631 (17)
β (°)	100.902 (3)
V (Å^3)	1914.8 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.20 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.705, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	52418, 3512, 2630
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.604
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.128, 1.05
No. of reflections	3512
No. of parameters	257
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, −0.22

Computer programs: *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x191469 [https://doi.org/10.1107/S241431461901469X]

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Bis{[2-(4-hydroxy-1*H*-indol-3-yl)ethyl]bis(propan-2-yl)azanium} but-2-enedioate tetrahydrate

Crystal data

$C_{16}H_{25}N_2O^+ \cdot 0.5C_4H_2O_4^{2-} \cdot 2H_2O$
M_r = 354.44
Monoclinic, $P2_1/n$
a = 8.3495 (8) Å
b = 12.5138 (11) Å
c = 18.6631 (17) Å
β = 100.902 (3)°
V = 1914.8 (3) Å^3
Z = 4
$F(000)$ = 768
D_x = 1.229 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9972 reflections
θ = 2.9–25.2°
μ = 0.09 mm^{-1}
T = 200 K
Shard, colourless
0.20 × 0.15 × 0.10 mm

Data collection

Bruker D8 Venture CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.705, T_{max} = 0.745
52418 measured reflections
3512 independent reflections
2630 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 25.4°, θ_{min} = 2.9°
h = −10→10
k = −15→15
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.128
S = 1.05
3512 reflections
257 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick 2018), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0155 (18)

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	0.94852 (17)	0.34667 (12)	0.25667 (7)	0.0394 (4)
O1W	0.5933 (3)	0.38719 (15)	0.16468 (15)	0.0764 (7)
O2	1.05696 (17)	0.46219 (12)	0.15852 (7)	0.0445 (4)
O2W	1.3681 (2)	0.53142 (15)	0.18964 (10)	0.0529 (5)
O3	0.82210 (18)	0.42826 (13)	0.08492 (7)	0.0457 (4)
N1	1.0659 (3)	0.16741 (15)	0.47495 (10)	0.0494 (5)
N2	0.60593 (19)	0.17587 (13)	0.19118 (8)	0.0321 (4)
C1	0.9055 (3)	0.15399 (17)	0.44334 (11)	0.0468 (6)
H1B	0.829526	0.112646	0.463512	0.056*
C2	1.1400 (3)	0.23028 (15)	0.43090 (10)	0.0381 (5)
C3	1.3016 (3)	0.26370 (17)	0.43917 (12)	0.0459 (6)
H3	1.380626	0.244438	0.480779	0.055*
C4	1.3413 (3)	0.32549 (18)	0.38466 (13)	0.0457 (5)
H4	1.450484	0.349755	0.388895	0.055*
C5	1.2268 (2)	0.35418 (16)	0.32296 (11)	0.0390 (5)
H5	1.259699	0.396749	0.286160	0.047*
C6	1.0666 (2)	0.32147 (15)	0.31481 (10)	0.0312 (4)
C7	1.0205 (2)	0.25791 (14)	0.36961 (10)	0.0307 (4)
C8	0.8697 (3)	0.20820 (15)	0.37881 (10)	0.0347 (5)
C9	0.7111 (2)	0.21074 (16)	0.32523 (11)	0.0372 (5)
H9A	0.683386	0.285434	0.310371	0.045*
H9B	0.622912	0.181941	0.348408	0.045*
C10	0.7250 (2)	0.14395 (16)	0.25814 (10)	0.0346 (5)
H10A	0.836979	0.150899	0.248342	0.042*
H10B	0.707217	0.067836	0.268820	0.042*
C11	0.6625 (3)	0.13956 (16)	0.12321 (11)	0.0379 (5)
H11A	0.584190	0.165736	0.080225	0.045*
H11B	0.769365	0.173093	0.122033	0.045*
C12	0.6794 (3)	0.02060 (19)	0.11654 (13)	0.0560 (6)
H12A	0.573370	−0.013926	0.117888	0.067*
H12B	0.760009	−0.006282	0.158518	0.067*
C13	0.7340 (3)	−0.0092 (2)	0.04618 (13)	0.0572 (6)
H13A	0.736537	−0.087204	0.041736	0.086*
H13B	0.843254	0.019698	0.046637	0.086*
H13C	0.657436	0.020577	0.004669	0.086*
C14	0.4340 (2)	0.14425 (17)	0.19474 (11)	0.0397 (5)
H14A	0.410134	0.165611	0.242711	0.048*
H14B	0.424083	0.065534	0.190902	0.048*
C15	0.3094 (3)	0.1947 (2)	0.13503 (14)	0.0594 (7)
H15A	0.319125	0.273426	0.138887	0.071*
H15B	0.333208	0.173394	0.087045	0.071*
C16	0.1391 (3)	0.1631 (2)	0.13865 (15)	0.0615 (7)
H16A	0.063310	0.198177	0.099119	0.092*
H16B	0.114132	0.185071	0.185742	0.092*
H16C	0.127829	0.085439	0.133480	0.092*

C17	0.9662 (2)	0.45901 (15)	0.09626 (10)	0.0317 (4)
C18	1.0407 (2)	0.49612 (15)	0.03381 (10)	0.0338 (4)
H18	1.152918	0.515150	0.043346	0.041*
H1	0.991 (3)	0.383 (2)	0.2241 (15)	0.066 (8)*
H2WA	1.372 (4)	0.591 (3)	0.1719 (19)	0.098 (12)*
H2	0.604 (3)	0.254 (2)	0.1887 (13)	0.052 (6)*
H2WB	1.261 (4)	0.505 (2)	0.1751 (15)	0.081 (9)*
H1A	1.121 (3)	0.135 (2)	0.5147 (15)	0.065 (8)*
H1WA	0.527 (4)	0.435 (2)	0.1698 (15)	0.072 (9)*
H1WB	0.670 (4)	0.403 (2)	0.1439 (17)	0.079 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0337 (8)	0.0537 (9)	0.0303 (7)	−0.0009 (7)	0.0044 (6)	0.0130 (7)
O1W	0.0541 (12)	0.0389 (10)	0.149 (2)	0.0080 (9)	0.0516 (13)	0.0289 (11)
O2	0.0450 (9)	0.0619 (10)	0.0258 (7)	−0.0141 (7)	0.0043 (6)	0.0076 (7)
O2W	0.0432 (10)	0.0484 (10)	0.0669 (11)	−0.0053 (8)	0.0104 (8)	0.0144 (9)
O3	0.0415 (9)	0.0666 (10)	0.0289 (7)	−0.0133 (7)	0.0065 (6)	0.0004 (7)
N1	0.0745 (14)	0.0405 (10)	0.0264 (9)	−0.0074 (10)	−0.0074 (9)	0.0056 (8)
N2	0.0315 (9)	0.0300 (9)	0.0347 (9)	0.0010 (7)	0.0063 (7)	0.0043 (7)
C1	0.0688 (16)	0.0388 (12)	0.0337 (11)	−0.0109 (11)	0.0117 (11)	0.0017 (9)
C2	0.0538 (13)	0.0286 (10)	0.0275 (10)	0.0017 (9)	−0.0034 (9)	−0.0034 (8)
C3	0.0488 (13)	0.0375 (12)	0.0420 (12)	0.0037 (10)	−0.0155 (10)	−0.0067 (10)
C4	0.0338 (11)	0.0431 (12)	0.0560 (14)	0.0007 (9)	−0.0026 (10)	−0.0107 (11)
C5	0.0356 (11)	0.0388 (11)	0.0431 (12)	−0.0002 (9)	0.0092 (9)	−0.0007 (9)
C6	0.0344 (10)	0.0311 (10)	0.0273 (9)	0.0046 (8)	0.0040 (8)	−0.0014 (8)
C7	0.0387 (11)	0.0270 (9)	0.0248 (9)	0.0017 (8)	0.0022 (8)	−0.0034 (7)
C8	0.0467 (12)	0.0301 (10)	0.0277 (10)	−0.0028 (8)	0.0077 (8)	−0.0024 (8)
C9	0.0369 (11)	0.0380 (11)	0.0385 (11)	−0.0034 (9)	0.0119 (9)	−0.0001 (9)
C10	0.0323 (10)	0.0351 (10)	0.0342 (10)	0.0015 (8)	0.0004 (8)	0.0009 (8)
C11	0.0367 (11)	0.0412 (12)	0.0362 (11)	−0.0001 (9)	0.0079 (9)	0.0034 (9)
C12	0.0807 (18)	0.0428 (13)	0.0442 (13)	0.0013 (12)	0.0111 (12)	−0.0023 (10)
C13	0.0663 (16)	0.0562 (15)	0.0494 (14)	0.0061 (12)	0.0114 (12)	−0.0111 (12)
C14	0.0304 (11)	0.0446 (12)	0.0443 (12)	−0.0030 (9)	0.0078 (9)	0.0030 (10)
C15	0.0373 (12)	0.0812 (18)	0.0563 (15)	−0.0030 (12)	0.0004 (11)	0.0113 (13)
C16	0.0371 (13)	0.0743 (18)	0.0691 (17)	0.0007 (12)	0.0000 (11)	0.0053 (14)
C17	0.0417 (11)	0.0306 (10)	0.0229 (9)	−0.0014 (8)	0.0067 (8)	−0.0015 (8)
C18	0.0403 (11)	0.0343 (10)	0.0281 (9)	−0.0032 (9)	0.0100 (8)	−0.0014 (8)

Geometric parameters (Å, º)

O1—C6	1.358 (2)	C8—C9	1.501 (3)
O1—H1	0.88 (3)	C9—H9A	0.9900
O1W—H1WA	0.83 (3)	C9—H9B	0.9900
O1W—H1WB	0.83 (3)	C9—C10	1.528 (3)
O2—C17	1.262 (2)	C10—H10A	0.9900
O2W—H2WA	0.82 (4)	C10—H10B	0.9900

O2W—H2WB	0.94 (3)	C11—H11A	0.9900
O3—C17	1.243 (2)	C11—H11B	0.9900
N1—C1	1.368 (3)	C11—C12	1.503 (3)
N1—C2	1.367 (3)	C12—H12A	0.9900
N1—H1A	0.89 (3)	C12—H12B	0.9900
N2—C10	1.496 (2)	C12—C13	1.516 (3)
N2—C11	1.505 (3)	C13—H13A	0.9800
N2—C14	1.503 (2)	C13—H13B	0.9800
N2—H2	0.98 (2)	C13—H13C	0.9800
C1—H1B	0.9500	C14—H14A	0.9900
C1—C8	1.365 (3)	C14—H14B	0.9900
C2—C3	1.393 (3)	C14—C15	1.511 (3)
C2—C7	1.411 (3)	C15—H15A	0.9900
C3—H3	0.9500	C15—H15B	0.9900
C3—C4	1.368 (3)	C15—C16	1.489 (3)
C4—H4	0.9500	C16—H16A	0.9800
C4—C5	1.397 (3)	C16—H16B	0.9800
C5—H5	0.9500	C16—H16C	0.9800
C5—C6	1.380 (3)	C17—C18	1.495 (3)
C6—C7	1.406 (3)	C18—C18^{i}	1.319 (4)
C7—C8	1.443 (3)	C18—H18	0.9500

C6—O1—H1	109.9 (17)	C9—C10—H10A	108.9
H1WA—O1W—H1WB	118 (3)	C9—C10—H10B	108.9
H2WA—O2W—H2WB	108 (3)	H10A—C10—H10B	107.7
C1—N1—H1A	127.6 (17)	N2—C11—H11A	108.6
C2—N1—C1	109.18 (17)	N2—C11—H11B	108.6
C2—N1—H1A	122.8 (17)	H11A—C11—H11B	107.6
C10—N2—C11	111.00 (15)	C12—C11—N2	114.73 (17)
C10—N2—C14	112.47 (15)	C12—C11—H11A	108.6
C10—N2—H2	107.9 (13)	C12—C11—H11B	108.6
C11—N2—H2	105.5 (14)	C11—C12—H12A	109.4
C14—N2—C11	114.36 (15)	C11—C12—H12B	109.4
C14—N2—H2	105.0 (13)	C11—C12—C13	111.4 (2)
N1—C1—H1B	124.7	H12A—C12—H12B	108.0
C8—C1—N1	110.7 (2)	C13—C12—H12A	109.4
C8—C1—H1B	124.7	C13—C12—H12B	109.4
N1—C2—C3	130.15 (19)	C12—C13—H13A	109.5
N1—C2—C7	107.29 (19)	C12—C13—H13B	109.5
C3—C2—C7	122.55 (19)	C12—C13—H13C	109.5
C2—C3—H3	121.5	H13A—C13—H13B	109.5
C4—C3—C2	116.94 (19)	H13A—C13—H13C	109.5
C4—C3—H3	121.5	H13B—C13—H13C	109.5
C3—C4—H4	118.9	N2—C14—H14A	109.0
C3—C4—C5	122.3 (2)	N2—C14—H14B	109.0
C5—C4—H4	118.9	N2—C14—C15	112.81 (17)
C4—C5—H5	119.6	H14A—C14—H14B	107.8
C6—C5—C4	120.8 (2)	C15—C14—H14A	109.0

C6—C5—H5	119.6	C15—C14—H14B	109.0
O1—C6—C5	124.15 (18)	C14—C15—H15A	109.1
O1—C6—C7	117.10 (17)	C14—C15—H15B	109.1
C5—C6—C7	118.74 (17)	H15A—C15—H15B	107.8
C2—C7—C8	107.28 (17)	C16—C15—C14	112.7 (2)
C6—C7—C2	118.64 (18)	C16—C15—H15A	109.1
C6—C7—C8	134.07 (17)	C16—C15—H15B	109.1
C1—C8—C7	105.59 (18)	C15—C16—H16A	109.5
C1—C8—C9	128.06 (19)	C15—C16—H16B	109.5
C7—C8—C9	126.23 (16)	C15—C16—H16C	109.5
C8—C9—H9A	109.7	H16A—C16—H16B	109.5
C8—C9—H9B	109.7	H16A—C16—H16C	109.5
C8—C9—C10	109.90 (16)	H16B—C16—H16C	109.5
H9A—C9—H9B	108.2	O2—C17—C18	116.23 (17)
C10—C9—H9A	109.7	O3—C17—O2	124.05 (17)
C10—C9—H9B	109.7	O3—C17—C18	119.71 (16)
N2—C10—C9	113.40 (16)	C17—C18—H18	118.2
N2—C10—H10A	108.9	C18^{i}—C18—C17	123.6 (2)
N2—C10—H10B	108.9	C18^{i}—C18—H18	118.2
O1—C6—C7—C2	−179.92 (16)	C3—C2—C7—C6	0.1 (3)
O1—C6—C7—C8	1.6 (3)	C3—C2—C7—C8	178.94 (18)
O2—C17—C18—C18^{i}	−175.7 (2)	C3—C4—C5—C6	0.5 (3)
O3—C17—C18—C18^{i}	3.7 (4)	C4—C5—C6—O1	179.62 (18)
N1—C1—C8—C7	0.7 (2)	C4—C5—C6—C7	−0.4 (3)
N1—C1—C8—C9	176.85 (19)	C5—C6—C7—C2	0.1 (3)
N1—C2—C3—C4	178.8 (2)	C5—C6—C7—C8	−178.3 (2)
N1—C2—C7—C6	−178.92 (17)	C6—C7—C8—C1	178.2 (2)
N1—C2—C7—C8	−0.1 (2)	C6—C7—C8—C9	2.0 (3)
N2—C11—C12—C13	179.03 (18)	C7—C2—C3—C4	0.0 (3)
N2—C14—C15—C16	179.9 (2)	C7—C8—C9—C10	69.5 (2)
C1—N1—C2—C3	−178.4 (2)	C8—C9—C10—N2	−156.21 (16)
C1—N1—C2—C7	0.5 (2)	C10—N2—C11—C12	61.6 (2)
C1—C8—C9—C10	−105.9 (2)	C10—N2—C14—C15	168.58 (19)
C2—N1—C1—C8	−0.8 (3)	C11—N2—C10—C9	158.64 (16)
C2—C3—C4—C5	−0.3 (3)	C11—N2—C14—C15	−63.6 (2)
C2—C7—C8—C1	−0.4 (2)	C14—N2—C10—C9	−71.8 (2)
C2—C7—C8—C9	−176.62 (18)	C14—N2—C11—C12	−66.9 (2)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3^{ii}	0.89 (3)	2.08 (3)	2.926 (2)	157 (2)
N2—H2···O1*W*	0.98 (2)	1.73 (3)	2.689 (2)	168 (2)
O1—H1···O2	0.88 (3)	1.74 (3)	2.625 (2)	174 (3)

O1*W*—H1*WA*···O2*W*^{iii}	0.83 (3)	1.88 (3)	2.710 (3)	172 (3)
O1*W*—H1*WB*···O3	0.83 (3)	1.86 (3)	2.684 (3)	171 (3)
O2*W*—H2*WB*···O2	0.94 (3)	1.76 (3)	2.695 (2)	173 (3)
O2*W*—H2*WA*···*Cg*^{iv}	0.82 (4)	2.69 (4)	3.488 (2)	167 (3)

Symmetry codes: (ii) $x+1/2, -y+1/2, z+1/2$; (iii) $x-1, y, z$; (iv) $-x+5/2, y+1/2, -z+1/2$.