



IUCrData

ISSN 2414-3146

Cetylpyridinium bromide monohydrate: localization of H atoms

Kina Muller, Eric Cyriel Hosten and Richard Betz*

Nelson Mandela University, Summerstrand Campus, Department of Chemistry, University Way, Summerstrand, PO Box 77000, Port Elizabeth, 6031, South Africa. *Correspondence e-mail: richard.betz@mandela.ac.za

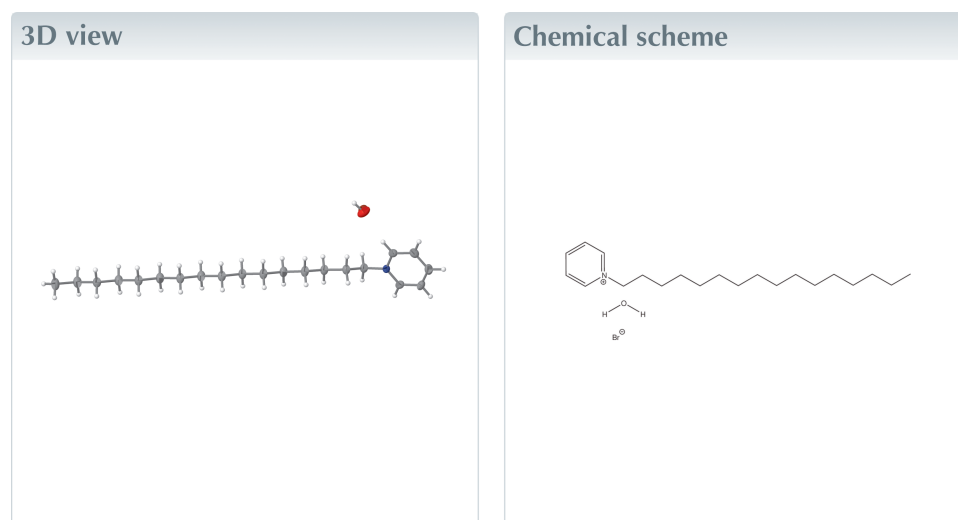
Received 6 November 2025

Accepted 7 November 2025

Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

Keywords: crystal structure; C—H...Br contacts; C—H...O contacts.**CCDC reference:** 2501304**Structural data:** full structural data are available from iucrdata.iucr.org

The title compound, $C_{21}H_{38}N^+ \cdot Br^- \cdot H_2O$, is the bromide salt of a quaternary pyridinium cation bearing a hexadecyl chain on the nitrogen atom. One molecule of solvent water is present in the asymmetric unit. Classical hydrogen bonds of the O—H...Br type are observed next to C—H...Br and C—H...O contacts that connect the entities of the title compound to sheets parallel to the *ab* plane.



Structure description

The effect of size and steric pretence of large ions on the chemical and spectroscopic properties of compounds have been a focus of research for many decades. Many effects can be attributed to the spatial requirements of counter-ions such as the glass-transition temperature in ionomers (Enokida *et al.*, 2020) or surfactant-modifying properties (Oh & Shah, 1993), the charge transfer in radical ions (Piotrowiak & Miller, 1993) and polymer-modified electrodes (Mathias & Haas, 1993) as well as the structural and vibrational spectroscopic behaviour of DNA building blocks (Minguirbara *et al.*, 2020). In addition, it has been found that selecting an adequate size of counter-ions to crystallize ionic compounds can be crucial for the isolation of crystalline reaction products of high quality, the latter having been confirmed and reviewed on many occasions (Roof & Kolis, 1993), with bis(triphenylphosphine)iminium being a good example for the successful crystallization of bulky transition-metal coordination compounds (McNicholas *et al.*, 2023). In a continuation of our interest in metrical features of large cations (Muller *et al.*, 2021*a,b,c,d,e,f,g*; Hosten *et al.*, 2012; Hosten *et al.*, 2015*a,b*; Hosten & Betz, 2024; Schoultz *et al.*, 2015), the structure of the title compound has been determined. While the latter has been reported previously (Ballirano *et al.*, 1998), no hydrogen-atom positions were determined, which precludes discussions of inter- and intramolecular interactions on a comparative basis in the envisioned ionic target compounds. The molecular and crystal structures of co-crystallizates of the title compound have been reported earlier (Iimura *et*



Published under a CC BY 4.0 licence

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1A \cdots Br1 ⁱ	0.84 (1)	2.49 (1)	3.3254 (14)	177 (2)
O1–H1B \cdots Br1	0.84 (1)	2.49 (1)	3.3227 (16)	171 (2)
C1–H1 \cdots Br1 ⁱⁱⁱ	0.95	2.87	3.5890 (17)	133
C3–H3 \cdots Br1 ⁱⁱⁱ	0.95	2.85	3.7797 (18)	168
C4–H4 \cdots O1 ^{iv}	0.95	2.59	3.362 (3)	138
C5–H5 \cdots O1	0.95	2.28	3.218 (2)	171
C6–H6B \cdots Br1	0.99	2.84	3.7702 (18)	156

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

al., 2002), as were the structures of the hydrated and anhydrous quinolinium equivalents (Wieckowski *et al.*, 2024). Furthermore, the molecular and crystal structures of two compounds featuring the title compound's cationic residue as leitmotif are apparent in the literature (Dalcanale *et al.*, 2021; Lu *et al.*, 2011). Cetylpyridinium bromide (CPB) as such has been employed extensively in germicidal applications, as well as in enzyme studies where CPB was used for polymerization, protein folding, gene delivery and, eventually, as a drug delivery agent in pharmaceuticals (Verma *et al.*, 2015; Ali *et al.*, 2023).

The structure solution shows the presence of an alkylated derivative of pyridine with the nitrogen atom bearing a hexadecyl chain. The positive charge of this pyridinium cation is counterbalanced by a bromide anion. Furthermore, a molecule of water is present in the asymmetric unit. The alkyl chain adopts an ideal zigzag conformation with all its carbon atoms being co-planar, and the largest deviation from the least-squares plane as defined by these carbon atoms measured at 0.026 (2) Å. The latter plane intersects with the least-squares plane as defined by the non-hydrogen atoms of the aromatic system at an angle of 60.30 (9)°. Intracyclic angles cover a range from 118.72 (17)–120.62 (17)° with the smallest angle on the carbon atom opposite from the pnictogen atom and the largest angle on one of the intracyclic carbon atoms directly bonded to the nitrogen atom (Fig. 1). Bond lengths are in good agreement with other alkylated pyridinium derivatives whose metrical parameters have been deposited with the Cambridge Structural Database (Groom *et al.*, 2016).

In the crystal structure, classical hydrogen bonds of the O–H \cdots Br type (Table 1) are observed next to C–H \cdots O as well as C–H \cdots Br contacts whose range falls by more than 0.1 Å below the sum of van der Waals radii of the atoms participating in them. The C–H \cdots O contacts are established

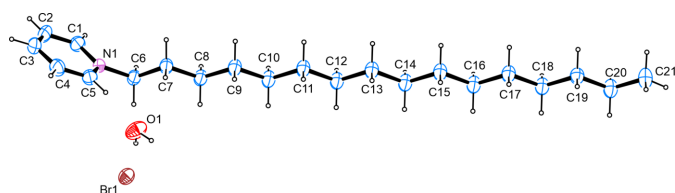


Figure 1
The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at the 50% probability level).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{38}N^+ \cdot Br^- \cdot H_2O$
M_r	402.45
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	200
a, b, c (Å)	5.5164 (2), 7.5140 (2), 27.3705 (9)
α, β, γ (°)	94.420 (1), 95.059 (1), 100.723 (1)
V (Å ³)	1105.28 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.87
Crystal size (mm)	0.44 × 0.29 × 0.03
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)
T_{min}, T_{max}	0.466, 0.511
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	49450, 4490, 4131
R_{int}	0.040
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.027, 0.062, 1.13
No. of reflections	4490
No. of parameters	226
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.33, -0.35

Computer programs: APEX2 and SAINT (Bruker, 2014), SHELXS97 (Sheldrick 2008), ORTEP-3 for Windows (Farrugia, 2012), Mercury (Macrae *et al.*, 2020), SHELXL2019/3 (Sheldrick, 2015) and PLATON (Spek, 2020).

by one of the aromatic CH groups in *ortho* position to the nitrogen atom as well as the adjacent aromatic CH group in the *meta* position to the pnictogen atom while the C–H \cdots Br contacts are observed between the second aromatic CH group in an *ortho* position to the nitrogen atom and the aromatic CH group in a *para* position as well as one of the hydrogen atoms of the methylene group directly bonded to the intracyclic heteroatom (Fig. 2). In total, the entities of the asymmetric unit are connected into a three-dimensional network. In terms of graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995), the classical hydrogen bonds require a DD descriptor on the unary level while the C–H \cdots O and C–H \cdots Br contacts necessitate a DDD descriptor on the same level. π -Stacking is not a prominent feature in the crystal structure of the title compound with the shortest intercentroid distance measured at 4.6493 (11) Å.

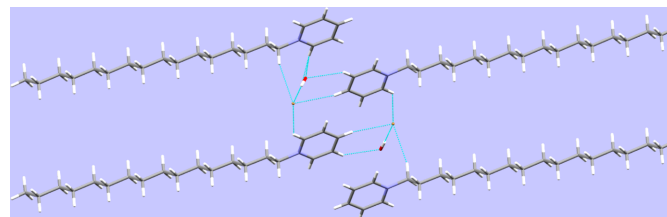


Figure 2
Selected intermolecular contacts, viewed along [010].

Synthesis and crystallization

The compound was obtained commercially (Fluka). Crystals suitable for the diffraction study were obtained upon recrystallization from boiling water.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The carbon-bound H atoms were placed in calculated positions ($C-H = 0.95 \text{ \AA}$ for the aromatic carbon atoms and $C-H = 0.99 \text{ \AA}$ for the methylene groups) and were included in the refinement in the riding model approximation, with $U_{iso}(H)$ set to $1.2U_{eq}(C)$. The H atoms of the methyl group were allowed to rotate with a fixed angle around the $C-C$ bond to best fit the experimental electron density [HFIX 137 in the *SHELX* program suite (Sheldrick, 2015)], with $U_{iso}(H)$ set to $1.5U_{eq}(C)$ and with $C-H = 0.98 \text{ \AA}$. The hydrogen atoms of the water molecule were located on a difference-Fourier map and refined freely with the $O-H$ distances restrained to $0.84(1) \text{ \AA}$ and the $H \cdots H$ distance restrained to $1.34(2) \text{ \AA}$.

References

- Ali, M. M., Hasan, T., Khan, J. M., Kumar, D., Ahmad, A., Rana, S., Rahman, M. M., Hoque, M. A. & Kabir, S. E. (2023). *RSC Adv.* **13**, 20709–20722.
- Ballirano, P., Caminiti, R., Sadun, C., Coiro, V. M., Mancini, G. & Maras, A. (1998). *Z. Kristallogr.* **213**, 123–129.
- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (2014). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Enokida, J. S., Hu, W., Fang, H., Morgan, B. F., Beyer, F. L., Winter, H. H. & Coughlin, E. B. (2020). *Macromolecules* **53**, 1767–1776.
- Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* **B46**, 256–262.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Hosten, E., Gerber, T. & Betz, R. (2012). *Z. Krist. New Cryst. Struct.* **227**, 331–332.
- Hosten, E., Schalekamp, H. & Betz, R. (2015a). *Z. Krist. New Cryst. Struct.* **230**, 303–305.
- Hosten, E., Schalekamp, H. & Betz, R. (2015b). *Z. Krist. New Cryst. Struct.* **230**, 295–297.
- Hosten, E. C. & Betz, R. (2024). *IUCrData* **9**, x240831.
- Iimura, N., Hirata, H. & Ohashi, Y. (2002). *Bull. Chem. Soc. Jpn* **75**, 71–75.
- Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
- Lu, J.-T., Lee, C.-K. & Lin, I. J. B. (2011). *Soft Matter* **7**, 3491–3501.
- Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
- Mathias, M. F. & Haas, O. (1993). *J. Phys. Chem.* **97**, 9217–9225.
- McNicholas, B. J., Nie, C., Jose, A., Oyala, P. H., Takase, M. K., Henling, L. M., Barth, A. T., Amaolo, A., Hadt, R. G., Solomon, E. I., Winkler, J. R., Gray, H. B. & Despagnet-Ayoub, E. (2023). *Inorg. Chem.* **62**, 2959–2981.
- Minguirbara, A., Vamhindi, B. S. D. R., Koyambo-Konzapa, S. J. & Nsangou, M. (2020). *J. Mol. Model.* **26** article No. 99.
- Muller, K., Hosten, E. C. & Betz, R. (2021a). *Z. Krist. New Cryst. Struct.* **236**, 353–355.
- Muller, K., Hosten, E. C. & Betz, R. (2021b). *Z. Krist. New Cryst. Struct.* **236**, 281–283.
- Muller, K., Hosten, E. C. & Betz, R. (2021c). *Z. Krist. New Cryst. Struct.* **236**, 285–286.
- Muller, K., Hosten, E. C. & Betz, R. (2021d). *Z. Krist. New Cryst. Struct.* **236**, 287–289.
- Muller, K., Hosten, E. C. & Betz, R. (2021e). *Z. Krist. New Cryst. Struct.* **236**, 335–337.
- Muller, K., Hosten, E. C. & Betz, R. (2021f). *Z. Krist. New Cryst. Struct.* **236**, 397–399.
- Muller, K., Hosten, E. C. & Betz, R. (2021g). *Z. Krist. New Cryst. Struct.* **236**, 301–303.
- Oh, S. G. & Shah, D. O. (1993). *J. Phys. Chem.* **97**, 284–286.
- Pedrini, A., Devi Das, A., Pinalli, R., Hickey, N., Geremia, S. & Dalcanale, E. (2021). *Eur. J. Org. Chem.* **2021**, 1547–1552.
- Piotrowiak, P. & Miller, J. R. (1993). *J. Phys. Chem.* **97**, 13052–13060.
- Roof, L. C. & Kolis, J. W. (1993). *Chem. Rev.* **93**, 1037–1080.
- Schoultz, X., Gerber, T. I. A., Hosten, E. C. & Betz, R. (2015). *Z. Krist. New Cryst. Struct.* **230**, 315–317.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Spek, A. L. (2020). *Acta Cryst.* **E76**, 1–11.
- Verma, R., Mishra, A. & Mitchell-Koch, K. R. (2015). *J. Chem. Theory Comput.* **11**, 5415–5425.
- Więckowski, M., Guńka, P., Świtalska, N. & Królikowski, M. (2024). *J. Mol. Liq.* **398**, 124191.

full crystallographic data

IUCrData (2025). **10**, x250991 [https://doi.org/10.1107/S2414314625009915]

Cetylpyridinium bromide monohydrate: localization of H atoms

Kina Muller, Eric Cyriel Hosten and Richard Betz

1-Hexadecylpyridin-1-ium bromide monohydrate

Crystal data

$C_{21}H_{38}N^+Br^- \cdot H_2O$

$M_r = 402.45$

Triclinic, $P\bar{1}$

$a = 5.5164$ (2) Å

$b = 7.5140$ (2) Å

$c = 27.3705$ (9) Å

$\alpha = 94.420$ (1)°

$\beta = 95.059$ (1)°

$\gamma = 100.723$ (1)°

$V = 1105.28$ (6) Å³

$Z = 2$

$F(000) = 432$

$D_x = 1.209$ Mg m⁻³

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

Cell parameters from 9771 reflections

$\theta = 2.3$ – 26.3 °

$\mu = 1.87$ mm⁻¹

$T = 200$ K

Platelet, colourless

$0.44 \times 0.29 \times 0.03$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.466$, $T_{\max} = 0.511$

49450 measured reflections

4490 independent reflections

4131 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 2.3$ °

$h = -6 \rightarrow 6$

$k = -9 \rightarrow 9$

$l = -34 \rightarrow 34$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.062$

$S = 1.13$

4490 reflections

226 parameters

3 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 0.5567P]$

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

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

$\Delta\rho_{\max} = 0.33$ e Å⁻³

$\Delta\rho_{\min} = -0.35$ 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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.28243 (3)	0.95301 (3)	0.12071 (2)	0.03558 (7)
O1	0.7091 (3)	0.7168 (2)	0.09060 (6)	0.0504 (4)
N1	0.0383 (2)	0.38072 (18)	0.10659 (5)	0.0266 (3)
C1	-0.1706 (3)	0.2569 (2)	0.09486 (7)	0.0339 (4)
H1	-0.279883	0.227204	0.119239	0.041*
C2	-0.2285 (4)	0.1725 (3)	0.04807 (7)	0.0409 (5)
H2	-0.378344	0.085771	0.039952	0.049*
C3	-0.0693 (4)	0.2135 (3)	0.01278 (7)	0.0401 (4)
H3	-0.108425	0.156670	-0.019922	0.048*
C4	0.1481 (4)	0.3385 (3)	0.02579 (7)	0.0390 (4)
H4	0.262145	0.367154	0.002180	0.047*
C5	0.1988 (3)	0.4213 (2)	0.07289 (7)	0.0339 (4)
H5	0.348200	0.507836	0.081857	0.041*
C6	0.0934 (3)	0.4768 (2)	0.15689 (6)	0.0311 (4)
H6A	-0.046325	0.435083	0.176244	0.037*
H6B	0.104912	0.608820	0.154518	0.037*
C7	0.3304 (3)	0.4468 (2)	0.18408 (6)	0.0314 (4)
H7A	0.473101	0.495722	0.166282	0.038*
H7B	0.324144	0.314736	0.185476	0.038*
C8	0.3644 (3)	0.5410 (2)	0.23604 (6)	0.0320 (4)
H8A	0.367090	0.672402	0.234064	0.038*
H8B	0.219492	0.491783	0.253230	0.038*
C9	0.5985 (3)	0.5194 (3)	0.26641 (6)	0.0337 (4)
H9A	0.743876	0.570106	0.249546	0.040*
H9B	0.596903	0.388158	0.268263	0.040*
C10	0.6273 (3)	0.6130 (3)	0.31830 (6)	0.0331 (4)
H10A	0.479346	0.564481	0.334707	0.040*
H10B	0.632261	0.744601	0.316285	0.040*
C11	0.8573 (3)	0.5898 (3)	0.34997 (6)	0.0336 (4)
H11A	1.005506	0.636551	0.333400	0.040*
H11B	0.851193	0.458422	0.352611	0.040*
C12	0.8855 (3)	0.6873 (3)	0.40158 (6)	0.0328 (4)
H12A	0.892594	0.818747	0.398871	0.039*
H12B	0.736422	0.641239	0.417977	0.039*
C13	1.1140 (3)	0.6639 (3)	0.43375 (6)	0.0336 (4)
H13A	1.106417	0.532484	0.436662	0.040*
H13B	1.263054	0.709292	0.417293	0.040*
C14	1.1420 (3)	0.7623 (3)	0.48512 (6)	0.0334 (4)
H14A	1.149548	0.893655	0.482182	0.040*
H14B	0.992850	0.716892	0.501544	0.040*
C15	1.3701 (3)	0.7392 (3)	0.51738 (6)	0.0337 (4)
H15A	1.519340	0.784577	0.500963	0.040*
H15B	1.362641	0.607804	0.520323	0.040*
C16	1.3980 (3)	0.8377 (3)	0.56876 (6)	0.0338 (4)
H16A	1.248828	0.792293	0.585183	0.041*

H16B	1.405644	0.969037	0.565828	0.041*
C17	1.6265 (3)	0.8144 (3)	0.60107 (6)	0.0337 (4)
H17A	1.619189	0.682963	0.603911	0.040*
H17B	1.775761	0.860093	0.584696	0.040*
C18	1.6542 (3)	0.9124 (3)	0.65253 (6)	0.0338 (4)
H18A	1.660006	1.043577	0.649665	0.041*
H18B	1.505536	0.865875	0.668984	0.041*
C19	1.8831 (3)	0.8908 (3)	0.68477 (6)	0.0328 (4)
H19A	1.876876	0.759561	0.687780	0.039*
H19B	2.031742	0.936616	0.668231	0.039*
C20	1.9115 (4)	0.9893 (3)	0.73601 (7)	0.0382 (4)
H20A	1.763700	0.942615	0.752705	0.046*
H20B	1.916372	1.120340	0.733038	0.046*
C21	2.1420 (4)	0.9684 (3)	0.76790 (7)	0.0460 (5)
H21A	2.137427	0.839242	0.771662	0.069*
H21B	2.147622	1.034676	0.800381	0.069*
H21C	2.289833	1.017933	0.752238	0.069*
H1A	0.852 (2)	0.778 (3)	0.0994 (9)	0.069 (8)*
H1B	0.614 (4)	0.784 (3)	0.1003 (10)	0.081 (10)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02816 (10)	0.03556 (11)	0.03999 (11)	0.00062 (7)	0.00212 (7)	-0.00012 (7)
O1	0.0321 (8)	0.0411 (8)	0.0731 (11)	-0.0018 (7)	0.0078 (7)	-0.0051 (7)
N1	0.0263 (7)	0.0260 (7)	0.0262 (7)	0.0042 (6)	-0.0031 (5)	0.0027 (6)
C1	0.0274 (9)	0.0337 (10)	0.0376 (10)	-0.0011 (7)	0.0003 (7)	0.0061 (8)
C2	0.0374 (10)	0.0383 (10)	0.0388 (10)	-0.0061 (8)	-0.0086 (8)	-0.0011 (8)
C3	0.0520 (12)	0.0367 (10)	0.0293 (9)	0.0095 (9)	-0.0061 (8)	-0.0021 (8)
C4	0.0429 (11)	0.0436 (11)	0.0303 (9)	0.0057 (9)	0.0049 (8)	0.0080 (8)
C5	0.0310 (9)	0.0341 (10)	0.0337 (9)	-0.0019 (7)	0.0016 (7)	0.0074 (7)
C6	0.0327 (9)	0.0313 (9)	0.0278 (9)	0.0067 (7)	-0.0015 (7)	-0.0016 (7)
C7	0.0321 (9)	0.0336 (9)	0.0276 (9)	0.0082 (7)	-0.0020 (7)	-0.0012 (7)
C8	0.0322 (9)	0.0347 (10)	0.0282 (9)	0.0089 (8)	-0.0018 (7)	-0.0035 (7)
C9	0.0325 (9)	0.0383 (10)	0.0294 (9)	0.0109 (8)	-0.0027 (7)	-0.0054 (7)
C10	0.0310 (9)	0.0394 (10)	0.0283 (9)	0.0103 (8)	-0.0011 (7)	-0.0042 (7)
C11	0.0325 (9)	0.0395 (10)	0.0282 (9)	0.0110 (8)	-0.0015 (7)	-0.0046 (7)
C12	0.0318 (9)	0.0388 (10)	0.0277 (9)	0.0107 (8)	-0.0008 (7)	-0.0032 (7)
C13	0.0317 (9)	0.0396 (10)	0.0290 (9)	0.0106 (8)	-0.0011 (7)	-0.0032 (7)
C14	0.0311 (9)	0.0400 (10)	0.0287 (9)	0.0103 (8)	-0.0007 (7)	-0.0037 (7)
C15	0.0319 (9)	0.0404 (10)	0.0285 (9)	0.0111 (8)	-0.0016 (7)	-0.0032 (7)
C16	0.0315 (9)	0.0407 (10)	0.0292 (9)	0.0115 (8)	-0.0008 (7)	-0.0035 (8)
C17	0.0323 (9)	0.0393 (10)	0.0292 (9)	0.0109 (8)	-0.0011 (7)	-0.0032 (7)
C18	0.0320 (9)	0.0402 (10)	0.0292 (9)	0.0108 (8)	-0.0004 (7)	-0.0022 (8)
C19	0.0326 (9)	0.0370 (10)	0.0293 (9)	0.0108 (8)	0.0003 (7)	-0.0014 (7)
C20	0.0370 (10)	0.0482 (11)	0.0294 (9)	0.0123 (9)	0.0001 (8)	-0.0028 (8)
C21	0.0429 (11)	0.0602 (13)	0.0324 (10)	0.0108 (10)	-0.0059 (8)	-0.0013 (9)

Geometric parameters (Å, °)

O1—H1A	0.837 (10)	C11—H11B	0.9900
O1—H1B	0.838 (10)	C12—C13	1.519 (2)
N1—C1	1.337 (2)	C12—H12A	0.9900
N1—C5	1.347 (2)	C12—H12B	0.9900
N1—C6	1.483 (2)	C13—C14	1.519 (2)
C1—C2	1.368 (3)	C13—H13A	0.9900
C1—H1	0.9500	C13—H13B	0.9900
C2—C3	1.376 (3)	C14—C15	1.517 (2)
C2—H2	0.9500	C14—H14A	0.9900
C3—C4	1.379 (3)	C14—H14B	0.9900
C3—H3	0.9500	C15—C16	1.519 (2)
C4—C5	1.369 (3)	C15—H15A	0.9900
C4—H4	0.9500	C15—H15B	0.9900
C5—H5	0.9500	C16—C17	1.520 (2)
C6—C7	1.509 (2)	C16—H16A	0.9900
C6—H6A	0.9900	C16—H16B	0.9900
C6—H6B	0.9900	C17—C18	1.520 (2)
C7—C8	1.519 (2)	C17—H17A	0.9900
C7—H7A	0.9900	C17—H17B	0.9900
C7—H7B	0.9900	C18—C19	1.517 (2)
C8—C9	1.515 (2)	C18—H18A	0.9900
C8—H8A	0.9900	C18—H18B	0.9900
C8—H8B	0.9900	C19—C20	1.516 (2)
C9—C10	1.517 (2)	C19—H19A	0.9900
C9—H9A	0.9900	C19—H19B	0.9900
C9—H9B	0.9900	C20—C21	1.518 (3)
C10—C11	1.518 (2)	C20—H20A	0.9900
C10—H10A	0.9900	C20—H20B	0.9900
C10—H10B	0.9900	C21—H21A	0.9800
C11—C12	1.522 (2)	C21—H21B	0.9800
C11—H11A	0.9900	C21—H21C	0.9800
H1A—O1—H1B	104.1 (18)	C13—C12—H12B	108.7
C1—N1—C5	120.59 (15)	C11—C12—H12B	108.7
C1—N1—C6	119.99 (15)	H12A—C12—H12B	107.6
C5—N1—C6	119.42 (14)	C14—C13—C12	113.91 (14)
N1—C1—C2	120.62 (17)	C14—C13—H13A	108.8
N1—C1—H1	119.7	C12—C13—H13A	108.8
C2—C1—H1	119.7	C14—C13—H13B	108.8
C1—C2—C3	119.91 (17)	C12—C13—H13B	108.8
C1—C2—H2	120.0	H13A—C13—H13B	107.7
C3—C2—H2	120.0	C15—C14—C13	114.07 (15)
C2—C3—C4	118.72 (17)	C15—C14—H14A	108.7
C2—C3—H3	120.6	C13—C14—H14A	108.7
C4—C3—H3	120.6	C15—C14—H14B	108.7
C5—C4—C3	119.71 (18)	C13—C14—H14B	108.7

C5—C4—H4	120.1	H14A—C14—H14B	107.6
C3—C4—H4	120.1	C14—C15—C16	114.04 (15)
N1—C5—C4	120.43 (16)	C14—C15—H15A	108.7
N1—C5—H5	119.8	C16—C15—H15A	108.7
C4—C5—H5	119.8	C14—C15—H15B	108.7
N1—C6—C7	113.70 (14)	C16—C15—H15B	108.7
N1—C6—H6A	108.8	H15A—C15—H15B	107.6
C7—C6—H6A	108.8	C15—C16—C17	114.01 (15)
N1—C6—H6B	108.8	C15—C16—H16A	108.8
C7—C6—H6B	108.8	C17—C16—H16A	108.8
H6A—C6—H6B	107.7	C15—C16—H16B	108.8
C6—C7—C8	110.07 (14)	C17—C16—H16B	108.8
C6—C7—H7A	109.6	H16A—C16—H16B	107.6
C8—C7—H7A	109.6	C18—C17—C16	114.06 (15)
C6—C7—H7B	109.6	C18—C17—H17A	108.7
C8—C7—H7B	109.6	C16—C17—H17A	108.7
H7A—C7—H7B	108.2	C18—C17—H17B	108.7
C9—C8—C7	114.14 (14)	C16—C17—H17B	108.7
C9—C8—H8A	108.7	H17A—C17—H17B	107.6
C7—C8—H8A	108.7	C19—C18—C17	114.24 (15)
C9—C8—H8B	108.7	C19—C18—H18A	108.7
C7—C8—H8B	108.7	C17—C18—H18A	108.7
H8A—C8—H8B	107.6	C19—C18—H18B	108.7
C8—C9—C10	113.24 (14)	C17—C18—H18B	108.7
C8—C9—H9A	108.9	H18A—C18—H18B	107.6
C10—C9—H9A	108.9	C20—C19—C18	114.25 (15)
C8—C9—H9B	108.9	C20—C19—H19A	108.7
C10—C9—H9B	108.9	C18—C19—H19A	108.7
H9A—C9—H9B	107.7	C20—C19—H19B	108.7
C9—C10—C11	114.38 (14)	C18—C19—H19B	108.7
C9—C10—H10A	108.7	H19A—C19—H19B	107.6
C11—C10—H10A	108.7	C19—C20—C21	113.96 (16)
C9—C10—H10B	108.7	C19—C20—H20A	108.8
C11—C10—H10B	108.7	C21—C20—H20A	108.8
H10A—C10—H10B	107.6	C19—C20—H20B	108.8
C10—C11—C12	113.63 (14)	C21—C20—H20B	108.8
C10—C11—H11A	108.8	H20A—C20—H20B	107.7
C12—C11—H11A	108.8	C20—C21—H21A	109.5
C10—C11—H11B	108.8	C20—C21—H21B	109.5
C12—C11—H11B	108.8	H21A—C21—H21B	109.5
H11A—C11—H11B	107.7	C20—C21—H21C	109.5
C13—C12—C11	114.11 (14)	H21A—C21—H21C	109.5
C13—C12—H12A	108.7	H21B—C21—H21C	109.5
C11—C12—H12A	108.7		
C5—N1—C1—C2	-1.7 (3)	C7—C8—C9—C10	-179.42 (16)
C6—N1—C1—C2	177.39 (16)	C8—C9—C10—C11	178.63 (16)
N1—C1—C2—C3	0.8 (3)	C9—C10—C11—C12	179.00 (16)

C1—C2—C3—C4	0.7 (3)	C10—C11—C12—C13	179.56 (16)
C2—C3—C4—C5	-1.2 (3)	C11—C12—C13—C14	179.66 (16)
C1—N1—C5—C4	1.2 (3)	C12—C13—C14—C15	179.98 (16)
C6—N1—C5—C4	-177.93 (16)	C13—C14—C15—C16	180.00 (16)
C3—C4—C5—N1	0.3 (3)	C14—C15—C16—C17	179.97 (16)
C1—N1—C6—C7	119.68 (18)	C15—C16—C17—C18	-179.82 (16)
C5—N1—C6—C7	-61.2 (2)	C16—C17—C18—C19	-179.52 (16)
N1—C6—C7—C8	-176.85 (14)	C17—C18—C19—C20	179.70 (16)
C6—C7—C8—C9	-179.81 (16)	C18—C19—C20—C21	-179.49 (17)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1A \cdots Br1 ⁱ	0.84 (1)	2.49 (1)	3.3254 (14)	177 (2)
O1—H1B \cdots Br1	0.84 (1)	2.49 (1)	3.3227 (16)	171 (2)
C1—H1 \cdots Br1 ⁱⁱ	0.95	2.87	3.5890 (17)	133
C3—H3 \cdots Br1 ⁱⁱⁱ	0.95	2.85	3.7797 (18)	168
C4—H4 \cdots O1 ^{iv}	0.95	2.59	3.362 (3)	138
C5—H5 \cdots O1	0.95	2.28	3.218 (2)	171
C6—H6B \cdots Br1	0.99	2.84	3.7702 (18)	156

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