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N-Benzyl-*N*-[2-(*N*-benzyl-*N*′,*N*′,*N*″,*N*″-tetramethylguanidiniumyl)ethyl]-*N*′,*N*′,*N*″,*N*″-tetramethylguanidinium dibromide 1.5-hydrate

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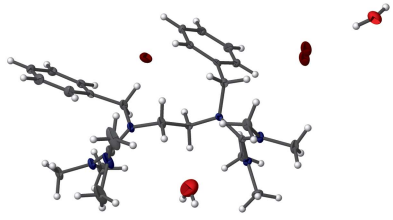
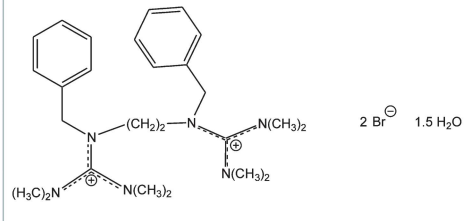
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the hydrated title compound, $C_{26}H_{42}N_6^{2+}\cdot 2Br^-\cdot 1.5H_2O$, comprises one cation, two bromide anions and one and a half water molecules, as one water molecule is fully occupied and the other is only half occupied [0.500 (6)]. Both bromide ions are disordered over two sites with refined occupancies of 0.938 (3):0.062 (3) and 0.520 (9):0.480 (9). The C—N bond lengths in both central C_3N units of the bisguanidinium ion range between 1.336 (3) and 1.349 (3) Å, indicating a degree of double-bond character. The central C atoms are bonded to the three N atoms in a nearly ideal trigonal–planar geometry and the positive charges are delocalized in both CN_3 planes. The crystal structure is stabilized by a three-dimensional network of O—H···O, O—H···Br and C—H···Br hydrogen bonds.

3D view



Chemical scheme



Structure description

By reaction of two equivalents of *N*,*N*,*N*′,*N*′-tetramethylchloroformamidinium chloride (Tiritiris & Kantlehner, 2008*a*) with 1,2-diaminoethane, a bisguanidinium dichloride (Wittmann *et al.*, 2000) has been obtained which, after treating with an aqueous sodium hydroxide solution, yields *N*,*N*,*N*′,*N*′-tetramethyl-*N*″-[2-(*N*′,*N*′,*N*″,*N*″-tetramethylguanidino)ethyl]guanidine (Tiritiris & Kantlehner, 2012). By alkylation of the free nitrogen atoms, various bisguanidinium salts can be prepared. The hydrated title salt presented here is the first alkylated bisguanidinium derivative in our series to have been structurally characterized. The asymmetric unit of the structure contains one cation, two bromide anions and one and a half water molecules (Fig. 1). Prominent bond parameters in the bisguanidinium cation are: C1—N1 = 1.336 (3), C1—N2 = 1.336 (3), C1—N3 =

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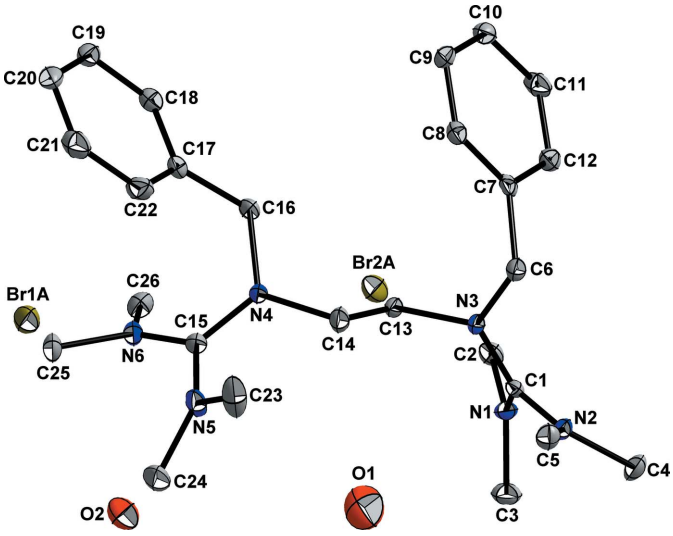

Figure 1
The structure of the title compound with displacement ellipsoids at the 50% probability level. All hydrogen atoms are omitted for the sake of clarity. Only the disordered bromine atoms with the major occupancy are shown.

1.349 (3) Å and C15—N4 = 1.349 (3), C15—N5 = 1.339 (3), C15—N6 = 1.339 (3) Å, indicating partial double-bond character for all. The N—C1—N and N—C15—N angles range from 119.4 (2)° to 120.4 (2)°, indicating that the carbon centres C1 and C15 adopt nearly ideal trigonal–planar environments. The positive charges of the dication are completely delocalized in both CN_3 planes. The crystal structure analysis reveals that the C—N and C—C bond lengths in the dication are in very good agreement with the values obtained for the diprotonated salt 1,2-bis-[2*N*′-(1,1,3,3-tetramethylguanidinium)]ethane dichloride tetrahydrate (Wittmann *et al.*, 2000). The crystal structure of the related *N*,*N*,*N*′,*N*′-tetramethyl-*N*′′-[2-(*N*′,*N*′,*N*′′,*N*′′- tetramethylguanidino)ethyl]guanidine, has also been reported (Tiritiris & Kantlehner, 2012).

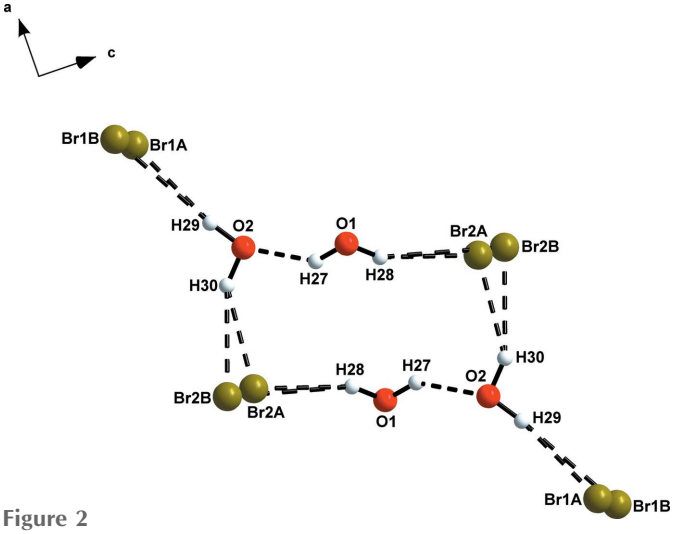

Figure 2
O—H···O and O—H···Br hydrogen bonds (black dashed lines) in the crystal structure of the title compound (view along *ac*).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H27···O2^{i}	0.89 (1)	1.87 (2)	2.646 (2)	146 (1)
O1—H28···Br2*A*^{ii}	0.89 (1)	2.31 (2)	3.160 (2)	159 (1)
O1—H28···Br2*B*^{ii}	0.89 (1)	2.90 (2)	3.720 (2)	155 (1)
O2—H29···Br1*A*	0.89 (1)	2.34 (2)	3.230 (2)	170 (1)
O2—H29···Br1*B*	0.89 (1)	2.75 (2)	3.637 (2)	173 (1)
O2—H30···Br2*A*^{iii}	0.90 (1)	2.39 (2)	3.139 (2)	141 (1)
O2—H30···Br2*B*^{iii}	0.90 (1)	2.52 (2)	3.346 (2)	153 (1)
C2—H2*B*···Br2*B*^{ii}	0.98	2.83	3.694 (2)	148
C3—H3*C*···Br2*A*^{ii}	0.98	2.87	3.634 (2)	136
C4—H4*C*···Br1*B*	0.98	2.85	3.632 (2)	137
C6—H6*A*···Br1*B*	0.99	2.64	3.611 (2)	169
C13—H13*A*···Br2*A*^{ii}	0.99	2.76	3.697 (2)	159
C13—H13*A*···Br2*B*^{ii}	0.99	2.84	3.804 (2)	165
C14—H14*B*···Br2*B*	0.99	2.81	3.692 (2)	149
C21—H21···Br1*B*^{iv}	0.95	2.90	3.544 (2)	126
C23—H23*A*···Br2*B*	0.98	2.73	3.525 (2)	138
C25—H25*A*···Br1*B*^{iv}	0.98	2.87	3.770 (2)	153
C26—H26*C*···Br2*B*^{ii}	0.98	2.84	3.641 (2)	139

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

The crystal structure is stabilized by a network of O—H···O, O—H···Br and C—H···Br hydrogen bonds, Table 1. O—H···O hydrogen bonds between the water molecules and O—H···Br hydrogen bonds between water molecules and bromide ions are observed, Fig. 2. In addition, C—H···Br hydrogen bonds form between the $-N(CH_3)_2$, $-CH_2$ and aromatic –CH groups of the cation and the bromide ions, forming a three-dimensional network, Fig. 3.

Synthesis and crystallization

The title compound was obtained by reaction of *N*,*N*,*N*′,*N*′-tetramethyl-*N*′′-[2-(*N*′,*N*′,*N*′′,*N*′′-tetramethylguanidino)ethyl]-guanidine (Tiritiris & Kantlehner, 2012) with two equivalents of benzyl bromide in acetonitrile at room temperature in nearly quantitative yield. After evaporation of the solvent, the

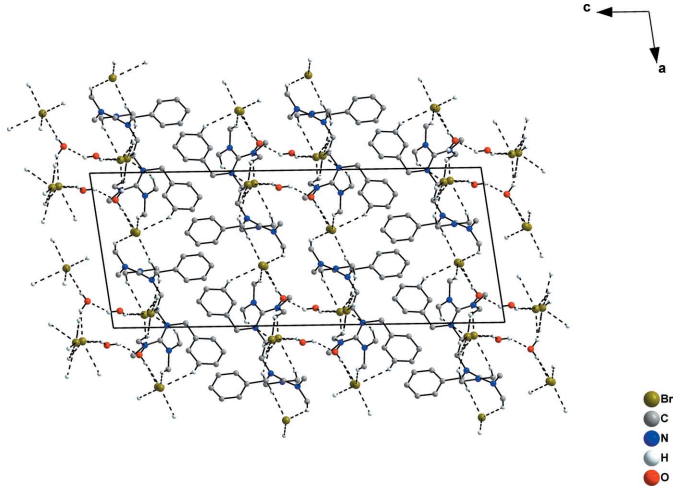

Figure 3
Molecular packing of the title compound. The O—H···O, O—H···Br and C—H···Br hydrogen bonds are depicted by black dashed lines (view in projection down the *b* axis).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{42}N_6^{2+}\cdot 2Br^-\cdot 1.5H_2O$
M_r	625.50
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	12.1957 (9), 7.9654 (5), 30.4821 (18)
β (°)	97.934 (4)
V (Å^3)	2932.8 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.80
Crystal size (mm)	0.35 × 0.26 × 0.10
Data collection	
Diffractometer	Bruker–Nonius KappaCCD diffractometer
Absorption correction	Multi-scan (Blessing, 1995)
T_{min}, T_{max}	0.455, 0.705
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11867, 7000, 5093
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.664
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.088, 1.02
No. of reflections	7000
No. of parameters	362
No. of restraints	5
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, −0.51

Computer programs: *COLLECT* (Hooft, 2004), *DENZO-SMN* (Otwinowski & Minor, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg & Putz, 2005).

crude product was recrystallized from a saturated acetonitrile-water solution. After several days at 273 K, colorless single crystals suitable for X-ray analysis were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atoms Br1 and Br2 are each disordered over two sites (Br1*A* and Br1*B*; Br2*A* and Br2*B*) with refined occupancy ratios of 0.938 (3):0.062 (3) and 0.520 (9):0.480 (9), respectively. The atoms Br1*A* and Br1*B* were restrained to have similar anisotropic displacement parameters. The position of O2 is only half occupied, the site occupancy factor was refined and converged to 0.500 (6). The occupancy factors of H29 and H30 were fixed to 0.5 and their U_{iso}(H) set at 0.050 Å^2.

Acknowledgements

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full crystallographic data

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N-Benzyl-*N*-[2-(*N*-benzyl-*N*′,*N*′,*N*′′,*N*′′-tetramethylguanidiniumyl)ethyl]-*N*′,*N*′,*N*′′,*N*′′-tetramethylguanidinium dibromide 1.5-hydrate

Crystal data

$C_{26}H_{42}N_6^{2+}\cdot 2Br^-\cdot 1.5H_2O$
M_r = 625.50
Monoclinic, $P2_1/c$
a = 12.1957 (9) Å
b = 7.9654 (5) Å
c = 30.4821 (18) Å
β = 97.934 (4)°
V = 2932.8 (3) Å^3
Z = 4
$F(000)$ = 1300
D_x = 1.417 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5843 reflections
θ = 0.4–28.3°
μ = 2.80 mm^{-1}
T = 100 K
Block, colorless
0.35 × 0.26 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ scans, and ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.455, T_{max} = 0.705
11867 measured reflections
7000 independent reflections
5093 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 28.1°, θ_{min} = 1.7°
h = −16→16
k = −10→9
l = −40→40

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.088
S = 1.02
7000 reflections
362 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 1.9458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1A	0.61652 (3)	0.32199 (15)	0.09074 (2)	0.02821 (18)	0.938 (3)
Br1B	0.6107 (5)	0.3919 (18)	0.0962 (2)	0.02821 (18)	0.062 (3)
Br2A	0.08222 (13)	0.1353 (4)	0.08416 (14)	0.0282 (5)	0.520 (9)
Br2B	0.08977 (8)	0.1763 (3)	0.10105 (14)	0.0240 (5)	0.480 (9)
C1	0.35370 (16)	0.7762 (3)	0.08670 (6)	0.0131 (5)	
N1	0.36249 (14)	0.9429 (2)	0.09049 (6)	0.0146 (4)	
N2	0.39307 (14)	0.6969 (2)	0.05355 (6)	0.0152 (4)	
N3	0.30713 (14)	0.6861 (2)	0.11675 (6)	0.0131 (4)	
C2	0.37669 (19)	1.0285 (3)	0.13337 (7)	0.0187 (5)	
H2A	0.3928	0.9456	0.1571	0.028*	
H2B	0.3086	1.0890	0.1371	0.028*	
H2C	0.4382	1.1084	0.1346	0.028*	
C3	0.3532 (2)	1.0538 (3)	0.05186 (7)	0.0224 (5)	
H3A	0.3354	0.9871	0.0248	0.034*	
H3B	0.4236	1.1123	0.0512	0.034*	
H3C	0.2944	1.1363	0.0537	0.034*	
C4	0.49080 (18)	0.7544 (3)	0.03505 (7)	0.0234 (5)	
H4A	0.5215	0.8537	0.0513	0.035*	
H4B	0.4700	0.7830	0.0037	0.035*	
H4C	0.5465	0.6649	0.0377	0.035*	
C5	0.34310 (18)	0.5430 (3)	0.03370 (7)	0.0192 (5)	
H5A	0.3905	0.4470	0.0435	0.029*	
H5B	0.3354	0.5517	0.0013	0.029*	
H5C	0.2699	0.5271	0.0429	0.029*	
C6	0.35329 (18)	0.5204 (3)	0.13192 (7)	0.0156 (5)	
H6A	0.4244	0.5016	0.1205	0.019*	
H6B	0.3014	0.4302	0.1203	0.019*	
C7	0.37139 (17)	0.5150 (3)	0.18194 (7)	0.0139 (5)	
C8	0.30142 (17)	0.4218 (3)	0.20481 (7)	0.0148 (5)	
H8	0.2453	0.3543	0.1888	0.018*	
C9	0.31251 (18)	0.4262 (3)	0.25082 (7)	0.0166 (5)	
H9	0.2646	0.3613	0.2661	0.020*	
C10	0.39372 (18)	0.5255 (3)	0.27427 (7)	0.0178 (5)	
H10	0.4000	0.5316	0.3056	0.021*	
C11	0.46563 (19)	0.6157 (3)	0.25182 (8)	0.0209 (5)	

H11	0.5224	0.6818	0.2678	0.025*	
C12	0.45473 (18)	0.6095 (3)	0.20599 (7)	0.0186 (5)	
H12	0.5049	0.6706	0.1908	0.022*	
C13	0.20801 (17)	0.7456 (3)	0.13420 (7)	0.0137 (4)	
H13A	0.1928	0.8635	0.1251	0.016*	
H13B	0.2204	0.7414	0.1670	0.016*	
C14	0.10851 (17)	0.6355 (3)	0.11665 (7)	0.0187 (5)	
H14A	0.0905	0.6512	0.0842	0.022*	
H14B	0.1278	0.5160	0.1223	0.022*	
C15	−0.08422 (18)	0.7306 (3)	0.11457 (7)	0.0202 (5)	
N4	0.01152 (14)	0.6780 (2)	0.13802 (5)	0.0158 (4)	
N5	−0.11477 (16)	0.6733 (3)	0.07340 (6)	0.0301 (5)	
N6	−0.15023 (15)	0.8373 (3)	0.13257 (6)	0.0196 (4)	
C16	0.02466 (18)	0.6553 (3)	0.18648 (7)	0.0180 (5)	
H16A	0.0436	0.7656	0.2005	0.022*	
H16B	0.0886	0.5799	0.1950	0.022*	
C17	−0.07320 (17)	0.5853 (3)	0.20581 (7)	0.0156 (5)	
C18	−0.08041 (18)	0.6212 (3)	0.24996 (7)	0.0173 (5)	
H18	−0.0277	0.6943	0.2659	0.021*	
C19	−0.16346 (18)	0.5518 (3)	0.27109 (7)	0.0195 (5)	
H19	−0.1663	0.5751	0.3015	0.023*	
C20	−0.24237 (19)	0.4481 (3)	0.24770 (7)	0.0230 (5)	
H20	−0.3000	0.4016	0.2619	0.028*	
C21	−0.23666 (19)	0.4129 (3)	0.20374 (8)	0.0253 (6)	
H21	−0.2910	0.3428	0.1876	0.030*	
C22	−0.15173 (19)	0.4794 (3)	0.18294 (7)	0.0214 (5)	
H22	−0.1474	0.4523	0.1529	0.026*	
C23	−0.0885 (2)	0.5048 (4)	0.05929 (9)	0.0488 (9)	
H23A	−0.0523	0.4414	0.0848	0.073*	
H23B	−0.0386	0.5123	0.0368	0.073*	
H23C	−0.1568	0.4475	0.0468	0.073*	
C24	−0.1789 (2)	0.7764 (5)	0.03946 (8)	0.0523 (10)	
H24A	−0.2551	0.7347	0.0340	0.078*	
H24B	−0.1456	0.7705	0.0120	0.078*	
H24C	−0.1789	0.8931	0.0496	0.078*	
C25	−0.27108 (18)	0.8224 (3)	0.12385 (8)	0.0260 (6)	
H25A	−0.2910	0.7196	0.1069	0.039*	
H25B	−0.3018	0.9199	0.1068	0.039*	
H25C	−0.3012	0.8176	0.1520	0.039*	
C26	−0.10728 (19)	0.9705 (3)	0.16283 (8)	0.0248 (6)	
H26A	−0.1106	0.9350	0.1934	0.037*	
H26B	−0.1520	1.0720	0.1564	0.037*	
H26C	−0.0303	0.9943	0.1591	0.037*	
O1	0.1101 (2)	0.8214 (4)	0.02327 (11)	0.0675 (7)	
H27	0.103 (4)	0.843 (5)	−0.0055 (4)	0.091 (17)*	
H28	0.088 (3)	0.916 (3)	0.0345 (12)	0.070 (14)*	
O2	0.8250 (3)	0.1418 (5)	0.05550 (12)	0.0313 (13)	0.500 (6)
H29	0.773 (3)	0.198 (7)	0.0678 (15)	0.050*	0.5

H30	0.885 (2)	0.150 (7)	0.0762 (13)	0.050*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1A	0.01796 (13)	0.0464 (5)	0.01941 (14)	−0.00219 (17)	−0.00051 (10)	−0.0025 (2)
Br1B	0.01796 (13)	0.0464 (5)	0.01941 (14)	−0.00219 (17)	−0.00051 (10)	−0.0025 (2)
Br2A	0.0256 (3)	0.0281 (6)	0.0315 (10)	0.0112 (3)	0.0065 (5)	0.0102 (7)
Br2B	0.0177 (3)	0.0254 (6)	0.0284 (10)	0.0038 (3)	0.0014 (4)	0.0068 (7)
C1	0.0094 (10)	0.0189 (12)	0.0102 (10)	−0.0001 (9)	−0.0013 (8)	0.0041 (9)
N1	0.0157 (9)	0.0169 (10)	0.0111 (8)	−0.0017 (8)	0.0012 (7)	0.0026 (8)
N2	0.0120 (9)	0.0228 (11)	0.0114 (8)	−0.0018 (8)	0.0037 (7)	−0.0028 (8)
N3	0.0115 (9)	0.0156 (10)	0.0129 (8)	0.0041 (8)	0.0047 (7)	0.0026 (8)
C2	0.0171 (11)	0.0213 (13)	0.0166 (11)	−0.0016 (10)	−0.0017 (9)	−0.0017 (10)
C3	0.0254 (13)	0.0223 (13)	0.0188 (12)	−0.0016 (11)	0.0006 (10)	0.0084 (10)
C4	0.0167 (11)	0.0382 (15)	0.0168 (11)	−0.0045 (11)	0.0070 (9)	−0.0015 (11)
C5	0.0169 (11)	0.0246 (13)	0.0159 (11)	−0.0004 (10)	0.0018 (9)	−0.0065 (10)
C6	0.0132 (10)	0.0173 (12)	0.0169 (11)	0.0019 (9)	0.0046 (9)	0.0010 (9)
C7	0.0112 (10)	0.0140 (11)	0.0160 (10)	0.0054 (9)	0.0004 (8)	0.0008 (9)
C8	0.0125 (10)	0.0133 (12)	0.0183 (11)	0.0011 (9)	0.0010 (9)	0.0010 (9)
C9	0.0137 (11)	0.0186 (12)	0.0182 (11)	−0.0014 (9)	0.0049 (9)	0.0040 (9)
C10	0.0180 (11)	0.0209 (13)	0.0141 (10)	0.0036 (10)	0.0006 (9)	0.0008 (10)
C11	0.0171 (11)	0.0221 (13)	0.0215 (11)	−0.0050 (10)	−0.0044 (9)	0.0034 (10)
C12	0.0138 (11)	0.0200 (12)	0.0219 (12)	−0.0010 (10)	0.0024 (9)	0.0073 (10)
C13	0.0133 (10)	0.0160 (11)	0.0126 (10)	0.0034 (9)	0.0043 (8)	0.0026 (9)
C14	0.0124 (10)	0.0281 (14)	0.0156 (11)	0.0027 (10)	0.0025 (9)	−0.0044 (10)
C15	0.0143 (11)	0.0340 (14)	0.0123 (10)	0.0045 (11)	0.0019 (9)	0.0025 (10)
N4	0.0100 (8)	0.0270 (11)	0.0105 (8)	0.0031 (8)	0.0019 (7)	0.0004 (8)
N5	0.0158 (10)	0.0607 (16)	0.0127 (9)	0.0124 (10)	−0.0019 (8)	−0.0083 (10)
N6	0.0116 (9)	0.0318 (12)	0.0153 (9)	0.0038 (9)	0.0019 (7)	−0.0015 (9)
C16	0.0119 (10)	0.0287 (14)	0.0125 (10)	−0.0006 (10)	−0.0013 (8)	0.0011 (10)
C17	0.0117 (10)	0.0179 (12)	0.0170 (11)	0.0039 (9)	0.0011 (8)	0.0030 (9)
C18	0.0158 (11)	0.0178 (12)	0.0175 (11)	0.0019 (10)	−0.0004 (9)	0.0015 (10)
C19	0.0210 (12)	0.0209 (13)	0.0173 (11)	0.0051 (10)	0.0056 (9)	0.0031 (10)
C20	0.0173 (12)	0.0276 (14)	0.0246 (12)	0.0005 (11)	0.0044 (10)	0.0110 (11)
C21	0.0183 (12)	0.0276 (14)	0.0279 (13)	−0.0070 (11)	−0.0042 (10)	0.0046 (11)
C22	0.0203 (12)	0.0285 (14)	0.0144 (11)	−0.0029 (11)	−0.0012 (9)	0.0001 (10)
C23	0.0229 (14)	0.087 (3)	0.0344 (16)	0.0087 (16)	−0.0034 (12)	−0.0379 (17)
C24	0.0231 (14)	0.118 (3)	0.0150 (12)	0.0198 (18)	−0.0010 (11)	0.0095 (16)
C25	0.0117 (11)	0.0438 (17)	0.0227 (12)	0.0056 (11)	0.0038 (9)	−0.0004 (12)
C26	0.0212 (12)	0.0340 (15)	0.0202 (12)	0.0023 (11)	0.0064 (10)	0.0007 (11)
O1	0.0614 (17)	0.0511 (18)	0.090 (2)	−0.0120 (14)	0.0107 (16)	0.0147 (17)
O2	0.027 (2)	0.029 (2)	0.036 (2)	0.0050 (17)	−0.0023 (16)	−0.0022 (17)

Geometric parameters (Å, º)

Br1A—Br1B	0.588 (14)	C14—H14A	0.9900
Br2A—Br2B	0.6061 (8)	C14—H14B	0.9900

C1—N1	1.336 (3)	C15—N4	1.349 (3)
C1—N2	1.336 (3)	C15—N5	1.339 (3)
C1—N3	1.349 (3)	C15—N6	1.339 (3)
N1—C2	1.463 (3)	N4—C16	1.475 (3)
N1—C3	1.464 (3)	N5—C23	1.459 (4)
N2—C4	1.461 (3)	N5—C24	1.460 (3)
N2—C5	1.463 (3)	N6—C26	1.455 (3)
N3—C13	1.465 (3)	N6—C25	1.466 (3)
N3—C6	1.484 (3)	C16—C17	1.509 (3)
C2—H2A	0.9800	C16—H16A	0.9900
C2—H2B	0.9800	C16—H16B	0.9900
C2—H2C	0.9800	C17—C22	1.389 (3)
C3—H3A	0.9800	C17—C18	1.390 (3)
C3—H3B	0.9800	C18—C19	1.388 (3)
C3—H3C	0.9800	C18—H18	0.9500
C4—H4A	0.9800	C19—C20	1.388 (3)
C4—H4B	0.9800	C19—H19	0.9500
C4—H4C	0.9800	C20—C21	1.380 (3)
C5—H5A	0.9800	C20—H20	0.9500
C5—H5B	0.9800	C21—C22	1.392 (3)
C5—H5C	0.9800	C21—H21	0.9500
C6—C7	1.511 (3)	C22—H22	0.9500
C6—H6A	0.9900	C23—H23A	0.9800
C6—H6B	0.9900	C23—H23B	0.9800
C7—C8	1.389 (3)	C23—H23C	0.9800
C7—C12	1.389 (3)	C24—H24A	0.9800
C8—C9	1.391 (3)	C24—H24B	0.9800
C8—H8	0.9500	C24—H24C	0.9800
C9—C10	1.386 (3)	C25—H25A	0.9800
C9—H9	0.9500	C25—H25B	0.9800
C10—C11	1.385 (3)	C25—H25C	0.9800
C10—H10	0.9500	C26—H26A	0.9800
C11—C12	1.386 (3)	C26—H26B	0.9800
C11—H11	0.9500	C26—H26C	0.9800
C12—H12	0.9500	O1—H27	0.89 (1)
C13—C14	1.532 (3)	O1—H28	0.89 (1)
C13—H13A	0.9900	O2—H29	0.89 (1)
C13—H13B	0.9900	O2—H30	0.90 (1)
C14—N4	1.467 (3)		

N2—C1—N1	120.15 (19)	N4—C14—H14A	109.4
N2—C1—N3	119.4 (2)	C13—C14—H14A	109.4
N1—C1—N3	120.40 (19)	N4—C14—H14B	109.4
C1—N1—C2	122.59 (18)	C13—C14—H14B	109.4
C1—N1—C3	122.27 (18)	H14A—C14—H14B	108.0
C2—N1—C3	115.08 (18)	N5—C15—N6	119.7 (2)
C1—N2—C4	122.81 (19)	N5—C15—N4	120.0 (2)
C1—N2—C5	122.44 (18)	N6—C15—N4	120.4 (2)

C4—N2—C5	114.73 (18)	C15—N4—C14	121.91 (18)
C1—N3—C13	121.39 (18)	C15—N4—C16	122.37 (18)
C1—N3—C6	120.50 (17)	C14—N4—C16	115.70 (16)
C13—N3—C6	118.08 (17)	C15—N5—C23	123.1 (2)
N1—C2—H2A	109.5	C15—N5—C24	121.7 (2)
N1—C2—H2B	109.5	C23—N5—C24	115.2 (2)
H2A—C2—H2B	109.5	C15—N6—C26	122.57 (19)
N1—C2—H2C	109.5	C15—N6—C25	121.4 (2)
H2A—C2—H2C	109.5	C26—N6—C25	116.04 (19)
H2B—C2—H2C	109.5	N4—C16—C17	117.00 (17)
N1—C3—H3A	109.5	N4—C16—H16A	108.0
N1—C3—H3B	109.5	C17—C16—H16A	108.0
H3A—C3—H3B	109.5	N4—C16—H16B	108.0
N1—C3—H3C	109.5	C17—C16—H16B	108.0
H3A—C3—H3C	109.5	H16A—C16—H16B	107.3
H3B—C3—H3C	109.5	C22—C17—C18	118.6 (2)
N2—C4—H4A	109.5	C22—C17—C16	123.8 (2)
N2—C4—H4B	109.5	C18—C17—C16	117.45 (19)
H4A—C4—H4B	109.5	C19—C18—C17	121.0 (2)
N2—C4—H4C	109.5	C19—C18—H18	119.5
H4A—C4—H4C	109.5	C17—C18—H18	119.5
H4B—C4—H4C	109.5	C20—C19—C18	119.8 (2)
N2—C5—H5A	109.5	C20—C19—H19	120.1
N2—C5—H5B	109.5	C18—C19—H19	120.1
H5A—C5—H5B	109.5	C21—C20—C19	119.7 (2)
N2—C5—H5C	109.5	C21—C20—H20	120.2
H5A—C5—H5C	109.5	C19—C20—H20	120.2
H5B—C5—H5C	109.5	C20—C21—C22	120.3 (2)
N3—C6—C7	109.64 (17)	C20—C21—H21	119.8
N3—C6—H6A	109.7	C22—C21—H21	119.8
C7—C6—H6A	109.7	C17—C22—C21	120.5 (2)
N3—C6—H6B	109.7	C17—C22—H22	119.8
C7—C6—H6B	109.7	C21—C22—H22	119.8
H6A—C6—H6B	108.2	N5—C23—H23A	109.5
C8—C7—C12	118.7 (2)	N5—C23—H23B	109.5
C8—C7—C6	120.48 (19)	H23A—C23—H23B	109.5
C12—C7—C6	120.8 (2)	N5—C23—H23C	109.5
C7—C8—C9	120.8 (2)	H23A—C23—H23C	109.5
C7—C8—H8	119.6	H23B—C23—H23C	109.5
C9—C8—H8	119.6	N5—C24—H24A	109.5
C10—C9—C8	119.8 (2)	N5—C24—H24B	109.5
C10—C9—H9	120.1	H24A—C24—H24B	109.5
C8—C9—H9	120.1	N5—C24—H24C	109.5
C11—C10—C9	119.8 (2)	H24A—C24—H24C	109.5
C11—C10—H10	120.1	H24B—C24—H24C	109.5
C9—C10—H10	120.1	N6—C25—H25A	109.5
C10—C11—C12	120.0 (2)	N6—C25—H25B	109.5
C10—C11—H11	120.0	H25A—C25—H25B	109.5

C12—C11—H11	120.0	N6—C25—H25C	109.5
C11—C12—C7	120.8 (2)	H25A—C25—H25C	109.5
C11—C12—H12	119.6	H25B—C25—H25C	109.5
C7—C12—H12	119.6	N6—C26—H26A	109.5
N3—C13—C14	109.99 (18)	N6—C26—H26B	109.5
N3—C13—H13A	109.7	H26A—C26—H26B	109.5
C14—C13—H13A	109.7	N6—C26—H26C	109.5
N3—C13—H13B	109.7	H26A—C26—H26C	109.5
C14—C13—H13B	109.7	H26B—C26—H26C	109.5
H13A—C13—H13B	108.2	H27—O1—H28	103 (4)
N4—C14—C13	111.17 (18)	H29—O2—H30	102.8 (15)

N2—C1—N1—C2	−147.57 (19)	N5—C15—N4—C14	32.3 (3)
N3—C1—N1—C2	31.1 (3)	N6—C15—N4—C14	−149.1 (2)
N2—C1—N1—C3	35.5 (3)	N5—C15—N4—C16	−146.1 (2)
N3—C1—N1—C3	−145.9 (2)	N6—C15—N4—C16	32.5 (3)
N1—C1—N2—C4	32.9 (3)	C13—C14—N4—C15	120.6 (2)
N3—C1—N2—C4	−145.7 (2)	C13—C14—N4—C16	−61.0 (3)
N1—C1—N2—C5	−148.7 (2)	N6—C15—N5—C23	−146.0 (2)
N3—C1—N2—C5	32.6 (3)	N4—C15—N5—C23	32.6 (4)
N2—C1—N3—C13	−140.3 (2)	N6—C15—N5—C24	33.1 (4)
N1—C1—N3—C13	41.0 (3)	N4—C15—N5—C24	−148.3 (2)
N2—C1—N3—C6	37.6 (3)	N5—C15—N6—C26	−145.8 (2)
N1—C1—N3—C6	−141.07 (19)	N4—C15—N6—C26	35.6 (3)
C1—N3—C6—C7	129.2 (2)	N5—C15—N6—C25	36.3 (3)
C13—N3—C6—C7	−52.8 (2)	N4—C15—N6—C25	−142.3 (2)
N3—C6—C7—C8	106.4 (2)	C15—N4—C16—C17	37.8 (3)
N3—C6—C7—C12	−70.5 (2)	C14—N4—C16—C17	−140.7 (2)
C12—C7—C8—C9	1.7 (3)	N4—C16—C17—C22	28.2 (3)
C6—C7—C8—C9	−175.2 (2)	N4—C16—C17—C18	−156.0 (2)
C7—C8—C9—C10	0.5 (3)	C22—C17—C18—C19	0.7 (3)
C8—C9—C10—C11	−2.0 (3)	C16—C17—C18—C19	−175.4 (2)
C9—C10—C11—C12	1.4 (4)	C17—C18—C19—C20	−1.6 (3)
C10—C11—C12—C7	0.8 (4)	C18—C19—C20—C21	1.0 (3)
C8—C7—C12—C11	−2.3 (3)	C19—C20—C21—C22	0.6 (4)
C6—C7—C12—C11	174.6 (2)	C18—C17—C22—C21	0.9 (3)
C1—N3—C13—C14	110.1 (2)	C16—C17—C22—C21	176.7 (2)
C6—N3—C13—C14	−67.8 (2)	C20—C21—C22—C17	−1.5 (4)
N3—C13—C14—N4	172.62 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H27···O2^{i}	0.89 (1)	1.87 (2)	2.646 (2)	146 (1)
O1—H28···Br2*A*^{ii}	0.89 (1)	2.31 (2)	3.160 (2)	159 (1)
O1—H28···Br2*B*^{ii}	0.89 (1)	2.90 (2)	3.720 (2)	155 (1)
O2—H29···Br1*A*	0.89 (1)	2.34 (2)	3.230 (2)	170 (1)
O2—H29···Br1*B*	0.89 (1)	2.75 (2)	3.637 (2)	173 (1)

O2—H30···Br2*A*^{iii}	0.90 (1)	2.39 (2)	3.139 (2)	141 (1)
O2—H30···Br2*B*^{iii}	0.90 (1)	2.52 (2)	3.346 (2)	153 (1)
C2—H2*B*···Br2*B*^{ii}	0.98	2.83	3.694 (2)	148
C3—H3*C*···Br2*A*^{ii}	0.98	2.87	3.634 (2)	136
C4—H4*C*···Br1*B*	0.98	2.85	3.632 (2)	137
C6—H6*A*···Br1*B*	0.99	2.64	3.611 (2)	169
C13—H13*A*···Br2*A*^{ii}	0.99	2.76	3.697 (2)	159
C13—H13*A*···Br2*B*^{ii}	0.99	2.84	3.804 (2)	165
C14—H14*B*···Br2*B*	0.99	2.81	3.692 (2)	149
C21—H21···Br1*B*^{iv}	0.95	2.90	3.544 (2)	126
C23—H23*A*···Br2*B*	0.98	2.73	3.525 (2)	138
C25—H25*A*···Br1*B*^{iv}	0.98	2.87	3.770 (2)	153
C26—H26*C*···Br2*B*^{ii}	0.98	2.84	3.641 (2)	139

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