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4-Methoxy-*N*,*N*′-diphenylbenzamidinium nitrate

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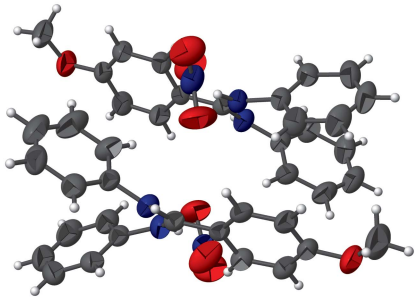
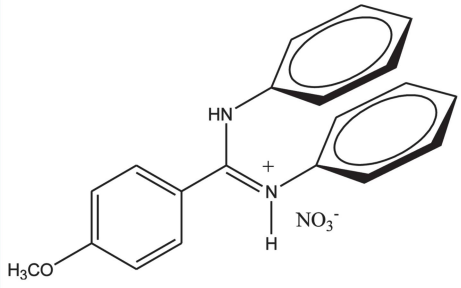
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title salt *N*,*N*′-diphenyl-4-methoxybenzamidinium nitrate, $C_{20}H_{19}N_2O^+\cdot NO_3^-$, comprises two independent *N*,*N*′-diphenyl-4-methoxybenzamidinium cations and two nitrate anions. The crystal structure features N—H···O hydrogen bonds and C—H···O contacts responsible for the packing.

3D view



Chemical scheme



Structure description

In the asymmetric unit of the title compound there are two independent *N*,*N*′-diphenyl-4-methoxy-benzamidinium cations (*A* and *B*) and two nitrate anions, as shown in Figs. 1 and 2. The protonation of the neutral amidine leads to important changes to the NCN moiety of the *N*,*N*′-diphenyl-4-methoxy-benzamidinium cation, with C—N bond lengths all close to 1.33 Å [C1*A*—N1*A* = 1.328 (4) Å, C1*A*—N2*A* = C1*B*—N1*B* = 1.324 (4) Å and C1*B*—N2*B* = 1.331 (3)]. By comparison, in the crystal structure of the neutral *N*,*N*′-diphenyl-4-methoxy-benzamidine, previously reported (Bortoluzzi *et al.*, 2004), two distinct C—N bond lengths, one short, 1.283 (2) Å (signifying C=N double-bond character) and one significantly longer, 1.372 (2) Å (commensurate with a single C—N bond). The maximum difference between the C—N bond lengths (Δ_{CN}) in the amidinium nitrate salt is only 0.011 Å, suggesting greater conjugation than in the neutral amidine, where the corresponding Δ_{CN} = 0.089 Å (Bortoluzzi *et al.*, 2004). The N—C—N and N—C—C bond angles in the amidinium moieties range from 117.5 (2) to 123.8 (3)° confirming the sp^2 character of the C1*A* and C1*B* atoms. This further corroborates the extensive conjugation in the NCN amidinium unit. The 4-methoxy-*N*-phenyl and amidinium moieties are almost coplanar in both the *A* and *B* molecules with torsion angles of −22.4 (4)° (N1*A*—C1*A*—C2*A*—C7*A*), 29.5 (4)° (N1*B*—C1*B*—C2*B*—C7*B*), 22.0 (4)° (N2*A*—C1*A*—C2*A*—C3*A*), and 32.9 (4)° (N2*B*—C1*B*—C2*B*—C3*B*). The 4-methoxy-*N*-phenyl and the two *N*-benzamidine ring planes are nearly orthogonal in molecule *B* [86.50 (9) and 88.20 (9)°], while in molecule *A* they are 74.77 (9) and 75.62 (9)°, respectively.

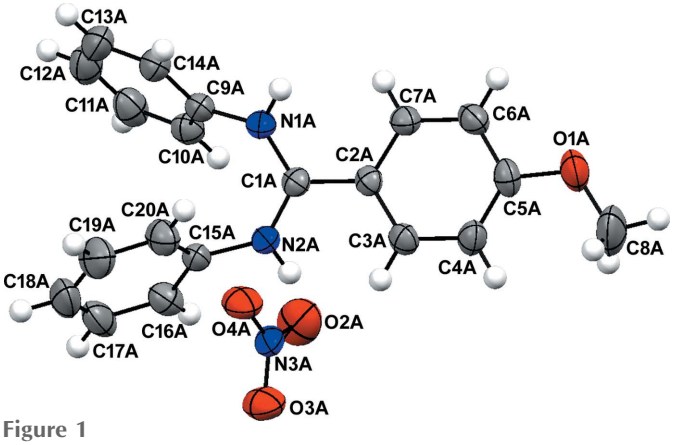


Figure 1
The molecular structure of the first ion pair in the title compound. Displacement ellipsoids are drawn at the 40% probability level.

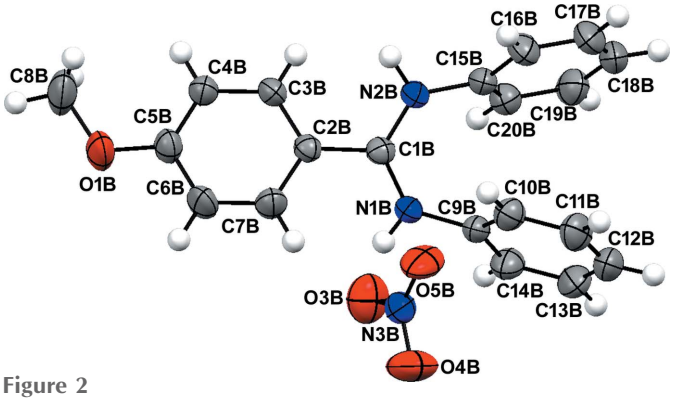


Figure 2
The molecular structure of the second ion pair in the title compound. Displacement ellipsoids are drawn at the 40% probability level.

In the crystal, N—H···O and N—H···(O,O) hydrogen bonds (Table 1) link the components into [100] chains of alternating cations and anions, as shown in Fig. 3. The packing is consolidated by C—H···O contacts.

Synthesis and crystallization

The preparation of *N*,*N*′-diphenyl-4-methoxy-benzamidine was performed according to the method described elsewhere (Bortoluzzi *et al.*, 2004). The nitrate salt was obtained by mixing equimolar ethanolic solutions of nitric acid and *N*,*N*′-diphenyl-4-methoxy-benzamidine at room temperature for 2 h. In a few days, colourless needle single crystals were obtained and filtered off. Additional characterization: m.p. 128–130°C); IR (ATR): 3370, 3190, 2937, 2843, 1626, 1602, 1581, 1554, 1516, 1491, 1373, 1330, 1309, 1257, 1190, 1047, 1022, 868, 754, 688 cm^{-1}. The strong band at 3190 cm^{-1} is assigned to the N—H stretching in the hydrogen-bonded amidinium-nitrate (N—H···O) system. The weak bands at 1373, 1330 and 1047 are tentatively assigned to the ν_3 and ν_1 nitrate vibrations in a hydrogen-bonded C_{2v} point group.

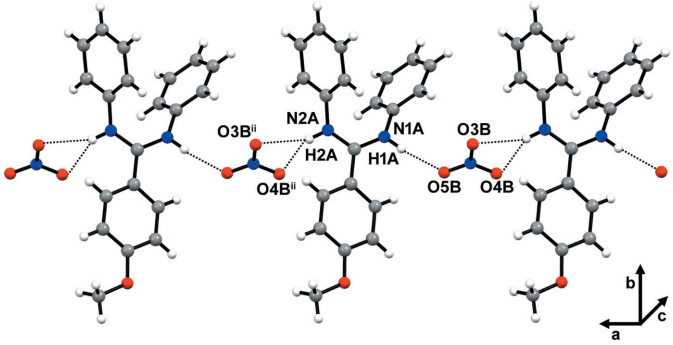


Figure 3
Details of the crystal packing showing the supramolecular chain formed by the hydrogen-bonding network. [Symmetry code: (ii) $x+1, y, z$.]

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1A···O5B	0.87 (3)	2.00 (3)	2.838 (4)	160 (3)
N1B—H1B···O2A^{i}	0.87 (3)	2.45 (3)	3.214 (4)	148 (3)
N1B—H1B···O3A^{i}	0.87 (3)	2.01 (3)	2.804 (4)	151 (3)
N1B—H1B···N3A^{i}	0.87 (3)	2.59 (3)	3.431 (4)	165 (3)
N2A—H2A···O3B^{ii}	0.84 (3)	2.20 (3)	3.006 (4)	160 (3)
N2A—H2A···O4B^{ii}	0.84 (3)	2.41 (3)	3.110 (4)	140 (3)
N2A—H2A···N3B^{ii}	0.84 (3)	2.69 (3)	3.506 (4)	163 (3)
N2B—H2B···O4A	0.95 (4)	1.88 (4)	2.798 (3)	161 (3)
C20B—H20B···O3A^{iii}	0.93	2.49	3.288 (4)	144

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{19}N_2O^+\cdot NO_3^-$
M_r	365.38
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	8.9453 (6), 24.8813 (17), 17.3105 (11)
β (°)	103.135 (2)
V (Å^3)	3752.0 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.36 × 0.24 × 0.21
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.659, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11714, 7113, 4403
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.209, 1.03
No. of reflections	7036
No. of parameters	503
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.69, −0.29

Computer programs: *APEX2* and *SAINT* (Bruker 2012.), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

Refinement

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

Acknowledgements

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full crystallographic data

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4-Methoxy-*N*,*N*′-diphenylbenzamidinium nitrate

Crystal data

$C_{20}H_{19}N_2O^+\cdot NO_3^-$
M_r = 365.38
Monoclinic, $P2_1/n$
a = 8.9453 (6) Å
b = 24.8813 (17) Å
c = 17.3105 (11) Å
β = 103.135 (2)°
V = 3752.0 (4) Å^3
Z = 8
F(000) = 1536
D_x = 1.294 Mg m^{-3}
Melting point: 402 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7126 reflections
θ = 2.5–25.8°
μ = 0.09 mm^{-1}
T = 293 K
Block, colourless
0.36 × 0.24 × 0.21 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
T_{min} = 0.659, T_{max} = 0.745
11714 measured reflections
7113 independent reflections
4403 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.7°, θ_{min} = 2.4°
h = −10→10
k = −30→23
l = −20→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.209
S = 1.03
7036 reflections
503 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0824P)^2 + 2.7248P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N2A	0.7989 (3)	0.37589 (10)	0.79592 (15)	0.0477 (6)
N2B	0.3596 (3)	0.42303 (10)	0.55453 (14)	0.0472 (6)
N1A	0.5570 (3)	0.35693 (10)	0.81612 (15)	0.0500 (6)
O1B	0.2700 (3)	0.62172 (10)	0.77506 (14)	0.0800 (8)
N1B	0.1099 (3)	0.41057 (10)	0.57207 (16)	0.0510 (6)
O1A	0.6056 (3)	0.17070 (9)	0.57383 (15)	0.0818 (8)
O4A	0.6337 (3)	0.48135 (11)	0.57798 (18)	0.0836 (8)
O3A	0.8626 (3)	0.48148 (11)	0.56225 (18)	0.0855 (8)
N3B	0.1528 (3)	0.31588 (11)	0.79441 (16)	0.0568 (7)
C2A	0.6604 (3)	0.30014 (11)	0.72843 (16)	0.0426 (6)
O5B	0.2803 (3)	0.29768 (11)	0.7990 (2)	0.1005 (10)
C1A	0.6732 (3)	0.34595 (11)	0.78207 (16)	0.0439 (6)
N3A	0.7594 (3)	0.45868 (11)	0.58905 (17)	0.0591 (7)
C15B	0.3576 (3)	0.38825 (12)	0.48831 (17)	0.0478 (7)
C9B	0.0772 (3)	0.35765 (11)	0.54199 (18)	0.0486 (7)
O4B	0.0561 (3)	0.28941 (14)	0.8181 (2)	0.1065 (10)
C2B	0.2558 (3)	0.48531 (11)	0.63535 (15)	0.0420 (6)
C15A	0.8143 (3)	0.43056 (11)	0.82121 (16)	0.0469 (7)
C9A	0.5648 (3)	0.38266 (11)	0.89039 (17)	0.0496 (7)
C1B	0.2410 (3)	0.43739 (11)	0.58449 (16)	0.0423 (6)
C7A	0.5594 (3)	0.25777 (12)	0.73282 (18)	0.0514 (7)
H7A	0.5026	0.2582	0.7716	0.062*
O3B	0.1133 (4)	0.35961 (11)	0.76528 (19)	0.1012 (10)
C3B	0.3441 (3)	0.52909 (12)	0.62266 (16)	0.0477 (7)
H3B	0.3977	0.5275	0.5826	0.057*
O2A	0.7876 (4)	0.41745 (12)	0.62410 (19)	0.1081 (11)
C4B	0.3533 (4)	0.57487 (12)	0.66859 (17)	0.0531 (7)
H4B	0.4141	0.6036	0.6598	0.064*
C3A	0.7485 (4)	0.29716 (12)	0.67163 (17)	0.0520 (7)
H3A	0.8174	0.3246	0.6684	0.062*
C20B	0.2472 (4)	0.39402 (13)	0.41896 (18)	0.0572 (8)
H20B	0.1743	0.4212	0.4135	0.069*
C10B	0.1730 (4)	0.31529 (12)	0.5716 (2)	0.0584 (8)
H10B	0.2582	0.3206	0.6131	0.070*
C7B	0.1763 (4)	0.48893 (13)	0.69605 (19)	0.0598 (8)
H7B	0.1181	0.4600	0.7064	0.072*
C10A	0.6878 (4)	0.37420 (13)	0.95373 (18)	0.0584 (8)
H10A	0.7710	0.3538	0.9469	0.070*
C6A	0.5436 (4)	0.21568 (12)	0.6804 (2)	0.0576 (8)
H6A	0.4743	0.1883	0.6829	0.069*
C5A	0.6310 (4)	0.21391 (12)	0.62346 (18)	0.0567 (8)
C4A	0.7351 (4)	0.25428 (12)	0.62014 (19)	0.0596 (8)
H4A	0.7961	0.2526	0.5833	0.072*
C5B	0.2723 (4)	0.57808 (12)	0.72751 (17)	0.0554 (8)
C14A	0.4422 (4)	0.41288 (13)	0.9002 (2)	0.0638 (9)

H14A	0.3591	0.4188	0.8578	0.077*
C20A	0.7020 (4)	0.46773 (13)	0.7925 (2)	0.0690 (9)
H20A	0.6114	0.4574	0.7576	0.083*
C14B	−0.0524 (4)	0.34912 (14)	0.4839 (2)	0.0653 (9)
H14B	−0.1193	0.3774	0.4659	0.078*
C16A	0.9499 (4)	0.44621 (14)	0.87062 (19)	0.0643 (9)
H16A	1.0275	0.4213	0.8883	0.077*
C16B	0.4699 (4)	0.34992 (14)	0.4945 (2)	0.0656 (9)
H16B	0.5469	0.3473	0.5406	0.079*
C6B	0.1837 (4)	0.53497 (14)	0.7404 (2)	0.0683 (10)
H6B	0.1284	0.5372	0.7798	0.082*
C11A	0.6876 (5)	0.39592 (15)	1.0271 (2)	0.0752 (11)
H11A	0.7705	0.3900	1.0696	0.090*
C11B	0.1398 (5)	0.26471 (13)	0.5383 (2)	0.0718 (10)
H11B	0.2042	0.2360	0.5573	0.086*
C19B	0.2474 (4)	0.35803 (16)	0.3568 (2)	0.0725 (10)
H19B	0.1727	0.3609	0.3099	0.087*
C12B	0.0139 (5)	0.25647 (15)	0.4782 (2)	0.0730 (10)
H12B	−0.0053	0.2226	0.4552	0.088*
C13B	−0.0837 (4)	0.29793 (16)	0.4518 (2)	0.0756 (11)
H13B	−0.1715	0.2920	0.4122	0.091*
C18B	0.3564 (5)	0.31886 (15)	0.3647 (2)	0.0741 (11)
H18B	0.3542	0.2946	0.3236	0.089*
C17B	0.4679 (5)	0.31519 (15)	0.4320 (3)	0.0786 (11)
H17B	0.5438	0.2891	0.4362	0.094*
C13A	0.4439 (5)	0.43467 (15)	0.9749 (3)	0.0824 (12)
H13A	0.3614	0.4552	0.9822	0.099*
C17A	0.9700 (5)	0.49970 (17)	0.8940 (2)	0.0815 (12)
H17A	1.0609	0.5105	0.9282	0.098*
C12A	0.5663 (6)	0.42590 (17)	1.0374 (2)	0.0844 (12)
H12A	0.5665	0.4405	1.0869	0.101*
C18A	0.8582 (7)	0.53605 (17)	0.8672 (3)	0.0931 (14)
H18A	0.8716	0.5717	0.8833	0.112*
C01G	0.3710 (6)	0.66524 (16)	0.7702 (3)	0.0968 (14)
H01A	0.3576	0.6930	0.8065	0.145*
H01B	0.4752	0.6527	0.7837	0.145*
H01C	0.3482	0.6793	0.7172	0.145*
C19A	0.7252 (6)	0.52031 (16)	0.8162 (3)	0.0938 (14)
H19A	0.6493	0.5456	0.7972	0.113*
C8A	0.6977 (7)	0.16646 (18)	0.5163 (3)	0.1156 (18)
H8A1	0.6694	0.1346	0.4850	0.173*
H8A2	0.6811	0.1974	0.4823	0.173*
H8A3	0.8041	0.1645	0.5429	0.173*
H2A	0.879 (4)	0.3634 (12)	0.7843 (17)	0.053 (9)*
H1A	0.469 (4)	0.3412 (12)	0.7986 (16)	0.047 (8)*
H1B	0.031 (4)	0.4262 (13)	0.5838 (18)	0.057 (9)*
H2B	0.454 (5)	0.4415 (16)	0.575 (2)	0.090 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2A	0.0402 (14)	0.0433 (14)	0.0616 (15)	0.0014 (11)	0.0155 (12)	−0.0046 (11)
N2B	0.0379 (13)	0.0495 (14)	0.0553 (14)	0.0010 (11)	0.0130 (11)	−0.0097 (12)
N1A	0.0383 (14)	0.0540 (15)	0.0580 (15)	−0.0032 (12)	0.0121 (12)	−0.0098 (12)
O1B	0.120 (2)	0.0624 (15)	0.0703 (15)	−0.0161 (14)	0.0478 (15)	−0.0238 (12)
N1B	0.0408 (14)	0.0450 (14)	0.0715 (17)	−0.0002 (11)	0.0219 (12)	−0.0095 (12)
O1A	0.116 (2)	0.0496 (14)	0.0845 (17)	−0.0149 (13)	0.0332 (16)	−0.0200 (12)
O4A	0.0500 (14)	0.0763 (17)	0.127 (2)	−0.0007 (13)	0.0261 (14)	−0.0018 (16)
O3A	0.0590 (15)	0.0775 (17)	0.127 (2)	0.0092 (13)	0.0352 (15)	0.0114 (16)
N3B	0.0523 (16)	0.0511 (16)	0.0677 (17)	0.0038 (13)	0.0148 (13)	−0.0021 (13)
C2A	0.0419 (15)	0.0368 (14)	0.0474 (15)	0.0045 (12)	0.0068 (12)	0.0020 (12)
O5B	0.0414 (14)	0.0766 (18)	0.185 (3)	0.0080 (13)	0.0286 (16)	−0.0061 (19)
C1A	0.0408 (15)	0.0419 (15)	0.0481 (15)	0.0046 (12)	0.0084 (12)	0.0021 (12)
N3A	0.0411 (15)	0.0553 (17)	0.0824 (19)	0.0030 (13)	0.0171 (14)	−0.0172 (15)
C15B	0.0428 (16)	0.0493 (17)	0.0550 (17)	−0.0047 (13)	0.0185 (13)	−0.0084 (14)
C9B	0.0460 (16)	0.0418 (16)	0.0633 (18)	−0.0031 (13)	0.0232 (14)	−0.0053 (14)
O4B	0.0689 (18)	0.122 (3)	0.139 (3)	−0.0125 (17)	0.0453 (18)	0.019 (2)
C2B	0.0387 (14)	0.0441 (15)	0.0429 (14)	0.0030 (12)	0.0091 (12)	−0.0019 (12)
C15A	0.0525 (17)	0.0416 (15)	0.0503 (16)	−0.0056 (13)	0.0196 (14)	−0.0032 (13)
C9A	0.0525 (18)	0.0438 (16)	0.0559 (17)	−0.0064 (13)	0.0194 (14)	−0.0032 (13)
C1B	0.0368 (15)	0.0404 (15)	0.0488 (15)	0.0047 (12)	0.0083 (12)	0.0044 (12)
C7A	0.0455 (17)	0.0484 (17)	0.0621 (18)	−0.0007 (13)	0.0158 (14)	−0.0009 (14)
O3B	0.125 (3)	0.0621 (17)	0.112 (2)	0.0198 (16)	0.0188 (19)	0.0215 (16)
C3B	0.0469 (16)	0.0522 (17)	0.0477 (15)	−0.0011 (13)	0.0188 (13)	−0.0064 (13)
O2A	0.150 (3)	0.0688 (19)	0.117 (2)	0.0229 (18)	0.055 (2)	0.0376 (17)
C4B	0.0595 (19)	0.0490 (17)	0.0543 (17)	−0.0068 (14)	0.0204 (15)	−0.0057 (14)
C3A	0.0634 (19)	0.0389 (15)	0.0556 (17)	−0.0019 (14)	0.0177 (15)	0.0039 (13)
C20B	0.0551 (19)	0.0554 (19)	0.0619 (19)	−0.0003 (15)	0.0148 (16)	−0.0043 (15)
C10B	0.062 (2)	0.0495 (18)	0.0650 (19)	−0.0011 (15)	0.0175 (16)	0.0024 (15)
C7B	0.073 (2)	0.0535 (19)	0.0602 (19)	−0.0130 (16)	0.0296 (17)	−0.0028 (15)
C10A	0.065 (2)	0.0535 (18)	0.0591 (19)	−0.0076 (15)	0.0191 (16)	0.0049 (15)
C6A	0.0555 (19)	0.0435 (17)	0.074 (2)	−0.0072 (14)	0.0149 (16)	−0.0009 (15)
C5A	0.076 (2)	0.0370 (16)	0.0550 (17)	0.0007 (15)	0.0095 (16)	−0.0029 (14)
C4A	0.081 (2)	0.0431 (17)	0.0611 (19)	0.0029 (16)	0.0300 (17)	−0.0028 (15)
C5B	0.072 (2)	0.0507 (18)	0.0461 (16)	−0.0026 (16)	0.0182 (15)	−0.0074 (14)
C14A	0.063 (2)	0.0553 (19)	0.078 (2)	0.0001 (16)	0.0271 (18)	−0.0074 (17)
C20A	0.069 (2)	0.0470 (19)	0.092 (2)	0.0039 (16)	0.0203 (19)	0.0046 (18)
C14B	0.0459 (18)	0.061 (2)	0.088 (2)	−0.0001 (15)	0.0140 (17)	−0.0078 (18)
C16A	0.065 (2)	0.063 (2)	0.065 (2)	−0.0131 (17)	0.0125 (17)	0.0012 (16)
C16B	0.0525 (19)	0.067 (2)	0.080 (2)	0.0076 (16)	0.0208 (17)	−0.0148 (18)
C6B	0.092 (3)	0.067 (2)	0.0595 (19)	−0.0111 (19)	0.0441 (19)	−0.0130 (17)
C11A	0.100 (3)	0.069 (2)	0.056 (2)	−0.021 (2)	0.017 (2)	−0.0027 (18)
C11B	0.087 (3)	0.0420 (18)	0.092 (3)	0.0054 (17)	0.031 (2)	0.0024 (18)
C19B	0.076 (2)	0.080 (3)	0.061 (2)	−0.017 (2)	0.0153 (18)	−0.0188 (19)
C12B	0.076 (2)	0.055 (2)	0.096 (3)	−0.0142 (19)	0.037 (2)	−0.021 (2)
C13B	0.058 (2)	0.080 (3)	0.089 (3)	−0.0154 (19)	0.0175 (19)	−0.026 (2)

C18B	0.072 (2)	0.070 (2)	0.092 (3)	−0.019 (2)	0.040 (2)	−0.037 (2)
C17B	0.065 (2)	0.069 (2)	0.111 (3)	0.0023 (19)	0.039 (2)	−0.026 (2)
C13A	0.097 (3)	0.063 (2)	0.103 (3)	0.000 (2)	0.056 (3)	−0.013 (2)
C17A	0.103 (3)	0.075 (3)	0.071 (2)	−0.041 (2)	0.028 (2)	−0.020 (2)
C12A	0.123 (4)	0.070 (3)	0.071 (3)	−0.021 (3)	0.045 (3)	−0.016 (2)
C18A	0.131 (4)	0.051 (2)	0.113 (3)	−0.022 (3)	0.061 (3)	−0.021 (2)
C01G	0.151 (4)	0.062 (2)	0.088 (3)	−0.025 (3)	0.048 (3)	−0.028 (2)
C19A	0.102 (3)	0.050 (2)	0.139 (4)	0.012 (2)	0.047 (3)	0.003 (2)
C8A	0.184 (5)	0.077 (3)	0.103 (3)	−0.020 (3)	0.068 (4)	−0.041 (3)

Geometric parameters (Å, º)

N2A—C1A	1.324 (4)	C10B—H10B	0.9300
N2A—C15A	1.426 (4)	C7B—C6B	1.373 (4)
N2A—H2A	0.84 (3)	C7B—H7B	0.9300
N2B—C1B	1.331 (3)	C10A—C11A	1.380 (5)
N2B—C15B	1.433 (4)	C10A—H10A	0.9300
N2B—H2B	0.95 (4)	C6A—C5A	1.390 (5)
N1A—C1A	1.335 (4)	C6A—H6A	0.9300
N1A—C9A	1.424 (4)	C5A—C4A	1.380 (4)
N1A—H1A	0.87 (3)	C4A—H4A	0.9300
O1B—C5B	1.366 (4)	C5B—C6B	1.382 (4)
O1B—C01G	1.425 (5)	C14A—C13A	1.399 (5)
N1B—C1B	1.324 (4)	C14A—H14A	0.9300
N1B—C9B	1.421 (4)	C20A—C19A	1.372 (5)
N1B—H1B	0.87 (3)	C20A—H20A	0.9300
O1A—C5A	1.363 (4)	C14B—C13B	1.392 (5)
O1A—C8A	1.434 (5)	C14B—H14B	0.9300
O4A—N3A	1.233 (3)	C16A—C17A	1.391 (5)
O3A—N3A	1.259 (3)	C16A—H16A	0.9300
N3B—O5B	1.213 (3)	C16B—C17B	1.382 (5)
N3B—O3B	1.217 (3)	C16B—H16B	0.9300
N3B—O4B	1.229 (4)	C6B—H6B	0.9300
C2A—C3A	1.395 (4)	C11A—C12A	1.362 (6)
C2A—C7A	1.401 (4)	C11A—H11A	0.9300
C2A—C1A	1.458 (4)	C11B—C12B	1.365 (5)
N3A—O2A	1.190 (4)	C11B—H11B	0.9300
C15B—C16B	1.372 (4)	C19B—C18B	1.363 (5)
C15B—C20B	1.377 (4)	C19B—H19B	0.9300
C9B—C14B	1.368 (4)	C12B—C13B	1.361 (5)
C9B—C10B	1.381 (4)	C12B—H12B	0.9300
C2B—C3B	1.392 (4)	C13B—H13B	0.9300
C2B—C7B	1.399 (4)	C18B—C17B	1.354 (6)
C2B—C1B	1.470 (4)	C18B—H18B	0.9300
C15A—C16A	1.372 (4)	C17B—H17B	0.9300
C15A—C20A	1.373 (4)	C13A—C12A	1.371 (6)
C9A—C14A	1.372 (4)	C13A—H13A	0.9300
C9A—C10A	1.381 (4)	C17A—C18A	1.350 (6)

C7A—C6A	1.372 (4)	C17A—H17A	0.9300
C7A—H7A	0.9300	C12A—H12A	0.9300
C3B—C4B	1.381 (4)	C18A—C19A	1.367 (7)
C3B—H3B	0.9300	C18A—H18A	0.9300
C4B—C5B	1.381 (4)	C01G—H01A	0.9600
C4B—H4B	0.9300	C01G—H01B	0.9600
C3A—C4A	1.378 (4)	C01G—H01C	0.9600
C3A—H3A	0.9300	C19A—H19A	0.9300
C20B—C19B	1.400 (5)	C8A—H8A1	0.9600
C20B—H20B	0.9300	C8A—H8A2	0.9600
C10B—C11B	1.388 (5)	C8A—H8A3	0.9600

C1A—N2A—C15A	127.7 (3)	C4A—C5A—C6A	120.0 (3)
C1A—N2A—H2A	119 (2)	C3A—C4A—C5A	119.8 (3)
C15A—N2A—H2A	113 (2)	C3A—C4A—H4A	120.1
C1B—N2B—C15B	127.4 (2)	C5A—C4A—H4A	120.1
C1B—N2B—H2B	116 (2)	O1B—C5B—C4B	125.0 (3)
C15B—N2B—H2B	116 (2)	O1B—C5B—C6B	115.6 (3)
C1A—N1A—C9A	127.4 (3)	C4B—C5B—C6B	119.4 (3)
C1A—N1A—H1A	119.4 (19)	C9A—C14A—C13A	119.0 (4)
C9A—N1A—H1A	111.7 (19)	C9A—C14A—H14A	120.5
C5B—O1B—C01G	118.2 (3)	C13A—C14A—H14A	120.5
C1B—N1B—C9B	128.8 (3)	C19A—C20A—C15A	119.1 (4)
C1B—N1B—H1B	118 (2)	C19A—C20A—H20A	120.5
C9B—N1B—H1B	113 (2)	C15A—C20A—H20A	120.5
C5A—O1A—C8A	117.2 (3)	C9B—C14B—C13B	119.7 (3)
O5B—N3B—O3B	122.7 (3)	C9B—C14B—H14B	120.2
O5B—N3B—O4B	120.0 (3)	C13B—C14B—H14B	120.2
O3B—N3B—O4B	117.2 (3)	C15A—C16A—C17A	119.4 (4)
C3A—C2A—C7A	118.2 (3)	C15A—C16A—H16A	120.3
C3A—C2A—C1A	121.0 (3)	C17A—C16A—H16A	120.3
C7A—C2A—C1A	120.8 (3)	C15B—C16B—C17B	119.6 (3)
N2A—C1A—N1A	121.3 (3)	C15B—C16B—H16B	120.2
N2A—C1A—C2A	119.7 (3)	C17B—C16B—H16B	120.2
N1A—C1A—C2A	119.0 (3)	C7B—C6B—C5B	120.9 (3)
O2A—N3A—O4A	123.7 (3)	C7B—C6B—H6B	119.6
O2A—N3A—O3A	119.2 (3)	C5B—C6B—H6B	119.6
O4A—N3A—O3A	117.1 (3)	C12A—C11A—C10A	120.2 (4)
C16B—C15B—C20B	120.5 (3)	C12A—C11A—H11A	119.9
C16B—C15B—N2B	118.7 (3)	C10A—C11A—H11A	119.9
C20B—C15B—N2B	120.7 (3)	C12B—C11B—C10B	121.0 (3)
C14B—C9B—C10B	120.3 (3)	C12B—C11B—H11B	119.5
C14B—C9B—N1B	118.8 (3)	C10B—C11B—H11B	119.5
C10B—C9B—N1B	120.8 (3)	C18B—C19B—C20B	120.4 (3)
C3B—C2B—C7B	118.1 (3)	C18B—C19B—H19B	119.8
C3B—C2B—C1B	121.1 (2)	C20B—C19B—H19B	119.8
C7B—C2B—C1B	120.7 (3)	C13B—C12B—C11B	119.8 (3)
C16A—C15A—C20A	120.3 (3)	C13B—C12B—H12B	120.1

C16A—C15A—N2A	118.2 (3)	C11B—C12B—H12B	120.1
C20A—C15A—N2A	121.3 (3)	C12B—C13B—C14B	120.3 (3)
C14A—C9A—C10A	120.0 (3)	C12B—C13B—H13B	119.9
C14A—C9A—N1A	118.8 (3)	C14B—C13B—H13B	119.9
C10A—C9A—N1A	121.0 (3)	C17B—C18B—C19B	120.3 (3)
N1B—C1B—N2B	123.8 (3)	C17B—C18B—H18B	119.9
N1B—C1B—C2B	117.5 (2)	C19B—C18B—H18B	119.9
N2B—C1B—C2B	118.7 (2)	C18B—C17B—C16B	120.5 (3)
C6A—C7A—C2A	120.6 (3)	C18B—C17B—H17B	119.7
C6A—C7A—H7A	119.7	C16B—C17B—H17B	119.7
C2A—C7A—H7A	119.7	C12A—C13A—C14A	120.5 (4)
C4B—C3B—C2B	121.1 (3)	C12A—C13A—H13A	119.8
C4B—C3B—H3B	119.4	C14A—C13A—H13A	119.8
C2B—C3B—H3B	119.4	C18A—C17A—C16A	120.2 (4)
C3B—C4B—C5B	120.0 (3)	C18A—C17A—H17A	119.9
C3B—C4B—H4B	120.0	C16A—C17A—H17A	119.9
C5B—C4B—H4B	120.0	C11A—C12A—C13A	120.0 (4)
C4A—C3A—C2A	121.2 (3)	C11A—C12A—H12A	120.0
C4A—C3A—H3A	119.4	C13A—C12A—H12A	120.0
C2A—C3A—H3A	119.4	C17A—C18A—C19A	119.9 (4)
C15B—C20B—C19B	118.5 (3)	C17A—C18A—H18A	120.1
C15B—C20B—H20B	120.7	C19A—C18A—H18A	120.1
C19B—C20B—H20B	120.7	O1B—C01G—H01A	109.5
C9B—C10B—C11B	118.8 (3)	O1B—C01G—H01B	109.5
C9B—C10B—H10B	120.6	H01A—C01G—H01B	109.5
C11B—C10B—H10B	120.6	O1B—C01G—H01C	109.5
C6B—C7B—C2B	120.4 (3)	H01A—C01G—H01C	109.5
C6B—C7B—H7B	119.8	H01B—C01G—H01C	109.5
C2B—C7B—H7B	119.8	C18A—C19A—C20A	121.1 (4)
C11A—C10A—C9A	120.2 (3)	C18A—C19A—H19A	119.5
C11A—C10A—H10A	119.9	C20A—C19A—H19A	119.5
C9A—C10A—H10A	119.9	O1A—C8A—H8A1	109.5
C7A—C6A—C5A	120.2 (3)	O1A—C8A—H8A2	109.5
C7A—C6A—H6A	119.9	H8A1—C8A—H8A2	109.5
C5A—C6A—H6A	119.9	O1A—C8A—H8A3	109.5
O1A—C5A—C4A	124.4 (3)	H8A1—C8A—H8A3	109.5
O1A—C5A—C6A	115.6 (3)	H8A2—C8A—H8A3	109.5

C15A—N2A—C1A—N1A	−24.1 (4)	C8A—O1A—C5A—C4A	2.2 (5)
C15A—N2A—C1A—C2A	155.7 (3)	C8A—O1A—C5A—C6A	−177.7 (4)
C9A—N1A—C1A—N2A	−28.3 (4)	C7A—C6A—C5A—O1A	−179.4 (3)
C9A—N1A—C1A—C2A	151.9 (3)	C7A—C6A—C5A—C4A	0.7 (5)
C3A—C2A—C1A—N2A	−22.0 (4)	C2A—C3A—C4A—C5A	1.2 (5)
C7A—C2A—C1A—N2A	157.8 (3)	O1A—C5A—C4A—C3A	178.0 (3)
C3A—C2A—C1A—N1A	157.8 (3)	C6A—C5A—C4A—C3A	−2.1 (5)
C7A—C2A—C1A—N1A	−22.4 (4)	C01G—O1B—C5B—C4B	−7.3 (5)
C1B—N2B—C15B—C16B	−135.7 (3)	C01G—O1B—C5B—C6B	173.7 (4)
C1B—N2B—C15B—C20B	45.9 (4)	C3B—C4B—C5B—O1B	−178.3 (3)

C1B—N1B—C9B—C14B	−133.1 (3)	C3B—C4B—C5B—C6B	0.7 (5)
C1B—N1B—C9B—C10B	47.8 (5)	C10A—C9A—C14A—C13A	−0.1 (5)
C1A—N2A—C15A—C16A	145.9 (3)	N1A—C9A—C14A—C13A	174.9 (3)
C1A—N2A—C15A—C20A	−39.0 (4)	C16A—C15A—C20A—C19A	−2.2 (5)
C1A—N1A—C9A—C14A	149.4 (3)	N2A—C15A—C20A—C19A	−177.2 (3)
C1A—N1A—C9A—C10A	−35.7 (4)	C10B—C9B—C14B—C13B	−3.1 (5)
C9B—N1B—C1B—N2B	15.2 (5)	N1B—C9B—C14B—C13B	177.9 (3)
C9B—N1B—C1B—C2B	−163.9 (3)	C20A—C15A—C16A—C17A	2.6 (5)
C15B—N2B—C1B—N1B	19.6 (5)	N2A—C15A—C16A—C17A	177.8 (3)
C15B—N2B—C1B—C2B	−161.3 (3)	C20B—C15B—C16B—C17B	−3.1 (5)
C3B—C2B—C1B—N1B	−148.0 (3)	N2B—C15B—C16B—C17B	178.5 (3)
C7B—C2B—C1B—N1B	29.5 (4)	C2B—C7B—C6B—C5B	−1.6 (6)
C3B—C2B—C1B—N2B	32.9 (4)	O1B—C5B—C6B—C7B	179.7 (3)
C7B—C2B—C1B—N2B	−149.6 (3)	C4B—C5B—C6B—C7B	0.6 (5)
C3A—C2A—C7A—C6A	−2.6 (4)	C9A—C10A—C11A—C12A	−0.1 (5)
C1A—C2A—C7A—C6A	177.6 (3)	C9B—C10B—C11B—C12B	−0.9 (5)
C7B—C2B—C3B—C4B	0.0 (4)	C15B—C20B—C19B—C18B	−1.2 (5)
C1B—C2B—C3B—C4B	177.6 (3)	C10B—C11B—C12B—C13B	−2.1 (6)
C2B—C3B—C4B—C5B	−1.0 (5)	C11B—C12B—C13B—C14B	2.4 (6)
C7A—C2A—C3A—C4A	1.1 (4)	C9B—C14B—C13B—C12B	0.2 (6)
C1A—C2A—C3A—C4A	−179.1 (3)	C20B—C19B—C18B—C17B	−1.6 (6)
C16B—C15B—C20B—C19B	3.5 (5)	C19B—C18B—C17B—C16B	2.1 (6)
N2B—C15B—C20B—C19B	−178.1 (3)	C15B—C16B—C17B—C18B	0.2 (6)
C14B—C9B—C10B—C11B	3.5 (5)	C9A—C14A—C13A—C12A	0.0 (5)
N1B—C9B—C10B—C11B	−177.5 (3)	C15A—C16A—C17A—C18A	−1.1 (6)
C3B—C2B—C7B—C6B	1.2 (5)	C10A—C11A—C12A—C13A	−0.1 (6)
C1B—C2B—C7B—C6B	−176.3 (3)	C14A—C13A—C12A—C11A	0.1 (6)
C14A—C9A—C10A—C11A	0.2 (5)	C16A—C17A—C18A—C19A	−0.7 (6)
N1A—C9A—C10A—C11A	−174.7 (3)	C17A—C18A—C19A—C20A	1.1 (7)
C2A—C7A—C6A—C5A	1.7 (5)	C15A—C20A—C19A—C18A	0.4 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O5*B*	0.87 (3)	2.00 (3)	2.838 (4)	160 (3)
N1*B*—H1*B*···O2*A*^{i}	0.87 (3)	2.45 (3)	3.214 (4)	148 (3)
N1*B*—H1*B*···O3*A*^{i}	0.87 (3)	2.01 (3)	2.804 (4)	151 (3)
N1*B*—H1*B*···N3*A*^{i}	0.87 (3)	2.59 (3)	3.431 (4)	165 (3)
N2*A*—H2*A*···O3*B*^{ii}	0.84 (3)	2.20 (3)	3.006 (4)	160 (3)
N2*A*—H2*A*···O4*B*^{ii}	0.84 (3)	2.41 (3)	3.110 (4)	140 (3)
N2*A*—H2*A*···N3*B*^{ii}	0.84 (3)	2.69 (3)	3.506 (4)	163 (3)
N2*B*—H2*B*···O4*A*	0.95 (4)	1.88 (4)	2.798 (3)	161 (3)
C20*B*—H20*B*···O3*A*^{iii}	0.93	2.49	3.288 (4)	144

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