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N,*N*,*N*′,*N*′-Tetramethyl-*N*″-[2-(trimethylazanium-yl)ethyl]guanidinium bis(tetraphenylborate) acetone disolvate

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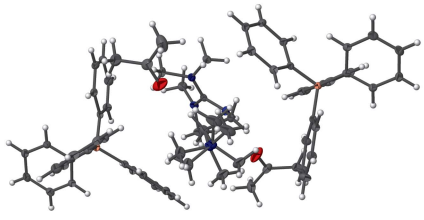
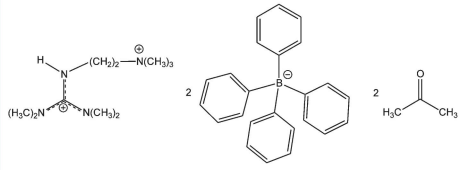
The asymmetric unit of the title solvated salt, $C_{10}H_{26}N_4^{2+}\cdot 2C_{24}H_{20}B^-\cdot 2C_3H_6O$, comprises one cation, two tetraphenylborate ions and two acetone solvent molecules. The N and methyl C atoms of the terminal trimethylammonium group are disordered over two sets of sites, with a refined occupancy ratio of 0.846 (3):0.154 (3). The C—N bond lengths in the central C_3N unit of the guanidinium ion range between 1.3308 (16) and 1.3508 (16) Å, indicating a degree of double-bond character. The central C atom is bonded to the three N atoms in a nearly ideal trigonal–planar geometry and the positive charge is delocalized in the CN_3 plane. The C—N bond lengths in the terminal trimethylammonium group have values close to that of a typical single bond, and the second positive charge is localized there. In the crystal, the guanidinium ion is connected by N—H···O and C—H···O hydrogen bonds with the acetone molecules. C—H···π interactions are present between the guanidinium H atoms and the phenyl rings of the tetraphenylborate ions, leading to the formation of a two-dimensional supramolecular pattern along the *bc* plane.

3D view



Chemical scheme



Structure description

ω-Aminoalkylguanidines like *N*″-[2-(dimethylamino)ethyl]- *N*,*N*,*N*′,*N*′-tetramethylguanidine (Tiritiris & Kantlehner, 2012) and its corresponding imine-nitrogen atom protonated guanidinium salts are well known in the literature (tetraphenylborate salt: Tiritiris & Kantlehner, 2012; bicarbonate salt: Tiritiris *et al.*, 2011). Electrophiles can attack on the nitrogen atom of the (dimethylamino)ethyl group in these salts. By alkylation of the chloride salt with one equivalent of dimethyl sulfate and after anion

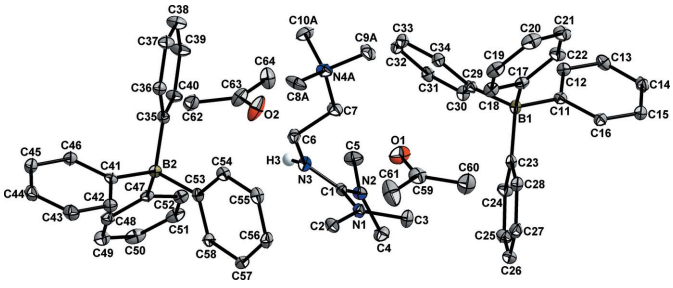


Figure 1
The structure of the title compound, with displacement ellipsoids at the 50% probability level. All H atoms (except for H3) have been omitted for the sake of clarity. Only the major population of the disordered $[NMe_3]^+$ group is shown.

exchange with sodium tetraphenylborate, the here-presented crystalline title compound emerged. The asymmetric unit of the structure comprises one cation, two tetraphenylborate ions and two acetone molecules (Fig. 1). The nitrogen and the methyl carbon atoms of the terminal trimethylammonium group are disordered over two sets of sites with a refined occupancy ratio of 0.846 (3):0.154 (3) (Fig. 2). Prominent bond parameters in the guanidinium ion are: C1—N1 = 1.3308 (16) Å, C1—N2 = 1.3425 (16) Å and C1—N3 = 1.3508 (16) Å, indicating partial double-bond character for all. The N—C1—N angles range from 118.36 (12) to 121.02 (11)°, indicating that the carbon centre C1 adopts a nearly ideal trigonal-planar environment. One of the two positive charges is completely delocalized in the CN_3 plane, while the second positive charge is localized at the terminal trimethylammonium group. The N—C bond lengths in the $[NMe_3]^+$ group have values close to a typical single bond [d(N—C) = 1.464 (17)–1.55 (3) Å].

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the C23–C28, C29–C34, C35–C40 and C53–C58 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O2	0.86 (2)	2.07 (2)	2.777 (2)	140 (2)
C9A—H9A3···O1	0.98	2.48	3.329 (2)	144
C8B—H8B1···O1	0.98	2.20	3.131 (2)	158
C7—H7A···O1	0.99	2.43	3.353 (2)	155
C3—H3C···*Cg*1	0.98	2.68	3.306 (2)	122
C9A—H9A1···*Cg*2^{i}	0.98	3.11	3.612 (2)	115
C9B—H9B2···*Cg*2^{i}	0.98	2.95	3.409 (2)	110
C10B—H10E···*Cg*3	0.98	2.48	3.337 (2)	146
C2—H2C···*Cg*4	0.98	2.98	3.543 (2)	108

Symmetry code: (i) $-x+1, -y, -z$.

The C—N and C—C bond lengths in the dication are in very good agreement with the values obtained for *N*,*N*,*N*′,*N*′-tetramethyl-*N*′′-[3-(trimethylazaniumyl)propyl]guanidinium bis(tetraphenylborate) acetone disolvate (Tiritiris, 2013*b*). The bond lengths and angles in both tetraphenylborate ions are in good agreement with the data from the crystal structure analysis of the alkali metal tetraphenylborates (Behrens *et al.*, 2012*a*).

In the crystal, the guanidinium ion is connected by N—H···O and C—H···O hydrogen bonds (Fig. 3) with the acetone molecules (Table 1). C—H···π interactions between the hydrogen atoms of –N(CH_3) groups of the guanidinium ion and the phenyl carbon atoms of the tetraphenylborate ions are present (Table 1). This leads to the formation of a two-dimensional supramolecular pattern along the *ac* plane (Fig. 4). Such C—H···π interactions have been also observed in *N*-[3-(benzyldimethylazaniumyl)propyl]-*N*′,*N*′,*N*′′,*N*′′-tetramethylguanidinium bis(tetraphenylborate) (Tiritiris, 2013*a*)

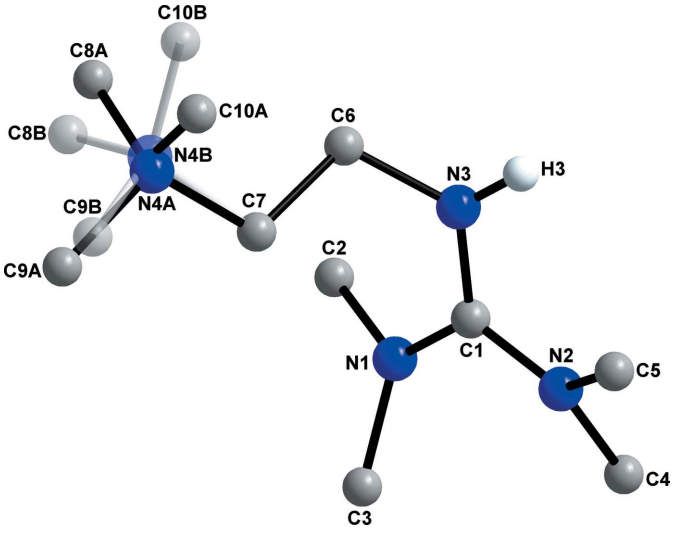


Figure 2
The structure of the guanidinium ion. All hydrogen atoms (except for H3) are omitted for the sake of clarity. The nitrogen and carbon atoms of the terminal $[NMe_3]^+$ group are disordered between the opaque (minor population) and dark (major population) positions.

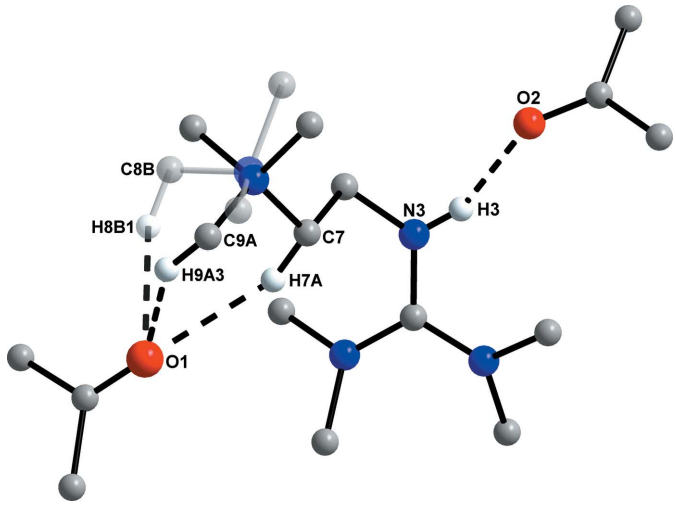


Figure 3
N—H···O and C—H···O hydrogen bonds (black dashed lines) between the guanidinium ion and the acetone molecules, including the minor population (opaque) and major population (dark) of the disordered $[NMe_3]^+$ group.

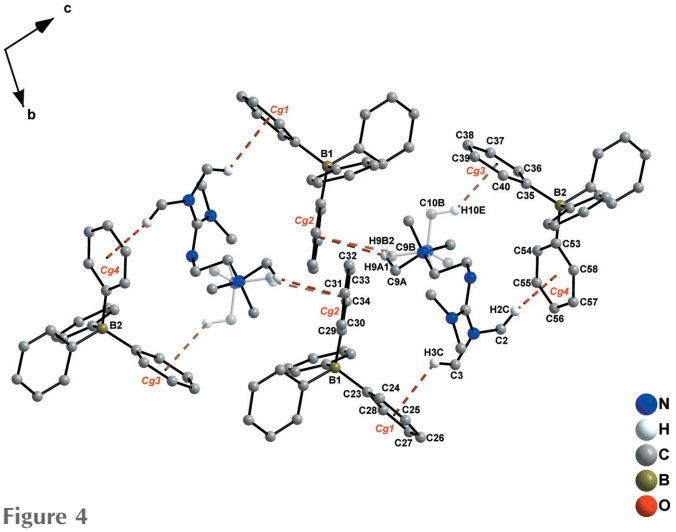


Figure 4
C—H···π interactions (brown dashed lines) between the hydrogen atoms of the guanidinium ion and the phenyl rings (centroids) of the tetraphenylborate ions (view along *bc*), including the minor population (opaque) and major population (dark) of the disordered $[NMe_3]^+$ group.

and *N*,*N*,*N*′,*N*′-tetramethyl-*N*″-[3-(trimethylazaniumyl)propyl]guanidinium bis(tetraphenylborate) acetone disolvate (Tiritiris, 2013*b*).

Synthesis and crystallization

The title compound was obtained by reaction of *N*,*N*,*N*′,*N*′-tetramethyl-*N*″-[2-(dimethylamino)ethyl]guanidinium chloride (Tiritiris & Kantlehner, 2012) with one equivalent of dimethyl sulfate in acetonitrile at room temperature. After evaporation of the solvent, the crude *N*,*N*,*N*′,*N*′-tetramethyl-*N*″-[2-(trimethylazaniumyl)ethyl]guanidinium chloride methyl sulfate (I) was washed with diethyl ether and dried *in vacuo*. 1.00 g (2.87 mmol) of (I) was dissolved in 20 ml acetonitrile and 1.96 g (5.74 mmol) of sodium tetraphenylborate in 20 ml acetonitrile was added. After stirring for one h at room temperature, the precipitated sodium chloride and sodium methyl sulfate was filtered off. The title compound crystallized from a saturated acetone solution after several weeks at 273 K, forming colorless single crystals. Yield: 2.18 g (88%).

Dimethyl sulfate is carcinogenic, mutagenic and highly poisonous. During the use appropriate precautions must be taken.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The The atoms N4, C8, C9 and C10 of the $[NMe_3]^+$ group are disordered over two sets of sites [N4*A*/N4*B*, C8*A*/C8*B*, C9*A*/C9*B* and C10*A*/C10*B*] with a refined occupancy ratio of 0.846 (3):0.154 (3). The two moieties were constrained to have similar geometries, and the anisotropic displacement parameters of equivalent atoms were constrained to be identical.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{26}N_4^{2+}\cdot 2C_{24}H_{20}B^-\cdot 2C_3H_6O$
M_r	956.92
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	11.4419 (3), 14.1461 (5), 18.8503 (9)
α, β, γ (°)	110.6352 (13), 101.824 (1), 97.8879 (8)
V (Å^3)	2720.70 (18)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.07
Crystal size (mm)	0.33 × 0.24 × 0.13
Data collection	
Diffractometer	Bruker–Nonius KappaCCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22310, 13295, 10609
R_{int}	0.021
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.050, 0.138, 1.02
No. of reflections	13295
No. of parameters	680
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.32

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

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full crystallographic data

IUCrData (2016). **1**, x160129 [https://doi.org/10.1107/S2414314616001292]

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N,*N*,*N*′,*N*′-Tetramethyl-*N*′′-[2-(trimethylazaniumyl)ethyl]guanidinium bis(tetraphenylborate) acetone disolvate

Crystal data

$C_{10}H_{26}N_4^{2+}\cdot 2C_{24}H_{20}B^-\cdot 2C_3H_6O$
M_r = 956.92
Triclinic, $P\overline{1}$
a = 11.4419 (3) Å
b = 14.1461 (5) Å
c = 18.8503 (9) Å
α = 110.6352 (13)°
β = 101.824 (1)°
γ = 97.8879 (8)°
V = 2720.70 (18) Å^3
Z = 2
$F(000)$ = 1032
D_x = 1.168 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 11355 reflections
θ = 0.4–28.3°
μ = 0.07 mm^{-1}
T = 100 K
Block, colorless
0.33 × 0.24 × 0.13 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ scans, and ω scans
22310 measured reflections
13295 independent reflections
10609 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 28.3°, θ_{min} = 1.2°
h = −15→15
k = −16→18
l = −24→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.138
S = 1.02
13295 reflections
680 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 1.2222P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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. 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 $F^2 > 2\text{sigma}(F^2)$ 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)
N1	0.59093 (10)	0.41666 (8)	0.31479 (6)	0.0158 (2)	
N2	0.75655 (10)	0.34377 (8)	0.34002 (6)	0.0160 (2)	
N3	0.56432 (10)	0.26444 (9)	0.33777 (7)	0.0160 (2)	
H3	0.5979 (17)	0.2332 (14)	0.3649 (11)	0.030 (5)*	
C1	0.63681 (11)	0.34267 (10)	0.33081 (7)	0.0142 (2)	
C2	0.48354 (12)	0.44848 (11)	0.33871 (8)	0.0182 (3)	
H2A	0.4108	0.4169	0.2933	0.027*	
H2B	0.4971	0.5242	0.3582	0.027*	
H2C	0.4710	0.4256	0.3806	0.027*	
C3	0.64100 (13)	0.46827 (11)	0.26869 (8)	0.0212 (3)	
H3A	0.6852	0.5396	0.3035	0.032*	
H3B	0.5738	0.4694	0.2276	0.032*	
H3C	0.6975	0.4303	0.2443	0.032*	
C4	0.85097 (12)	0.44027 (11)	0.37520 (8)	0.0213 (3)	
H4A	0.8133	0.4991	0.3947	0.032*	
H4B	0.8905	0.4479	0.3354	0.032*	
H4C	0.9125	0.4386	0.4191	0.032*	
C5	0.80177 (13)	0.24885 (11)	0.32670 (9)	0.0232 (3)	
H5A	0.8248	0.2398	0.3765	0.035*	
H5B	0.8736	0.2540	0.3063	0.035*	
H5C	0.7372	0.1892	0.2883	0.035*	
C6	0.43715 (11)	0.21537 (10)	0.29157 (7)	0.0170 (3)	
H6A	0.3835	0.2625	0.3101	0.020*	
H6B	0.4105	0.1506	0.2989	0.020*	
C7	0.42530 (12)	0.19057 (11)	0.20429 (8)	0.0208 (3)	
H7A	0.4279	0.2558	0.1955	0.025*	
H7B	0.4971	0.1640	0.1911	0.025*	
N4A	0.3105 (4)	0.1127 (3)	0.1488 (2)	0.0178 (4)	0.846 (3)
C8A	0.19893 (18)	0.1358 (2)	0.17388 (14)	0.0382 (6)	0.846 (3)
H8A1	0.2064	0.1348	0.2263	0.057*	0.846 (3)
H8A2	0.1265	0.0833	0.1362	0.057*	0.846 (3)
H8A3	0.1903	0.2045	0.1756	0.057*	0.846 (3)
C9A	0.29953 (19)	0.11284 (18)	0.06795 (11)	0.0304 (5)	0.846 (3)
H9A1	0.2325	0.0554	0.0295	0.046*	0.846 (3)
H9A2	0.3766	0.1045	0.0541	0.046*	0.846 (3)
H9A3	0.2824	0.1787	0.0676	0.046*	0.846 (3)
C10A	0.32390 (19)	0.00665 (14)	0.14393 (12)	0.0330 (5)	0.846 (3)
H10A	0.3262	0.0024	0.1949	0.049*	0.846 (3)
H10B	0.4002	−0.0059	0.1304	0.049*	0.846 (3)
H10C	0.2541	−0.0457	0.1033	0.049*	0.846 (3)

N4B	0.299 (2)	0.1157 (16)	0.1554 (13)	0.0178 (4)	0.154 (3)
C8B	0.2084 (11)	0.1796 (11)	0.1593 (8)	0.0382 (6)	0.154 (3)
H8B1	0.2325	0.2345	0.1412	0.057*	0.154 (3)
H8B2	0.2040	0.2109	0.2138	0.057*	0.154 (3)
H8B3	0.1279	0.1361	0.1255	0.057*	0.154 (3)
C9B	0.3109 (11)	0.0687 (10)	0.0737 (6)	0.0304 (5)	0.154 (3)
H9B1	0.3659	0.1193	0.0638	0.046*	0.154 (3)
H9B2	0.2300	0.0488	0.0360	0.046*	0.154 (3)
H9B3	0.3446	0.0071	0.0675	0.046*	0.154 (3)
C10B	0.2609 (11)	0.0254 (8)	0.1770 (7)	0.0330 (5)	0.154 (3)
H10D	0.1931	−0.0261	0.1340	0.049*	0.154 (3)
H10E	0.2342	0.0500	0.2252	0.049*	0.154 (3)
H10F	0.3305	−0.0064	0.1857	0.049*	0.154 (3)
B1	0.77548 (13)	0.27582 (11)	0.04141 (8)	0.0138 (3)	
C11	0.88932 (11)	0.27236 (9)	−0.00039 (7)	0.0136 (2)	
C12	0.95590 (11)	0.19452 (10)	−0.01608 (7)	0.0155 (2)	
H12	0.9370	0.1389	−0.0002	0.019*	
C13	1.04867 (12)	0.19517 (11)	−0.05401 (8)	0.0189 (3)	
H13	1.0916	0.1410	−0.0629	0.023*	
C14	1.07830 (12)	0.27478 (11)	−0.07873 (8)	0.0193 (3)	
H14	1.1417	0.2759	−0.1043	0.023*	
C15	1.01347 (12)	0.35294 (10)	−0.06543 (8)	0.0190 (3)	
H15	1.0316	0.4074	−0.0827	0.023*	
C16	0.92198 (12)	0.35140 (10)	−0.02680 (8)	0.0171 (3)	
H16	0.8797	0.4060	−0.0179	0.021*	
C17	0.64551 (12)	0.25013 (10)	−0.02617 (8)	0.0156 (2)	
C18	0.53451 (12)	0.26090 (10)	−0.00582 (8)	0.0181 (3)	
H18	0.5359	0.2833	0.0482	0.022*	
C19	0.42312 (12)	0.24021 (11)	−0.06130 (9)	0.0224 (3)	
H19	0.3509	0.2492	−0.0447	0.027*	
C20	0.41749 (13)	0.20643 (11)	−0.14102 (9)	0.0248 (3)	
H20	0.3418	0.1921	−0.1792	0.030*	
C21	0.52392 (14)	0.19396 (11)	−0.16378 (8)	0.0248 (3)	
H21	0.5211	0.1700	−0.2181	0.030*	
C22	0.63568 (13)	0.21642 (10)	−0.10724 (8)	0.0200 (3)	
H2	0.7076	0.2086	−0.1244	0.024*	
C23	0.80202 (11)	0.39532 (10)	0.10867 (7)	0.0144 (2)	
C24	0.90731 (12)	0.43503 (10)	0.17312 (8)	0.0195 (3)	
H24	0.9599	0.3903	0.1791	0.023*	
C25	0.93838 (13)	0.53692 (11)	0.22868 (8)	0.0223 (3)	
H25	1.0107	0.5599	0.2712	0.027*	
C26	0.86385 (13)	0.60503 (11)	0.22215 (8)	0.0215 (3)	
H26	0.8841	0.6745	0.2599	0.026*	
C27	0.75911 (13)	0.56894 (10)	0.15907 (8)	0.0199 (3)	
H27	0.7068	0.6141	0.1535	0.024*	
C28	0.73019 (12)	0.46676 (10)	0.10378 (8)	0.0166 (3)	
H28	0.6586	0.4446	0.0609	0.020*	
C29	0.77013 (11)	0.18967 (10)	0.08248 (7)	0.0146 (2)	

C30	0.87714 (12)	0.17699 (10)	0.12790 (8)	0.0170 (3)
H30	0.9530	0.2229	0.1379	0.020*
C31	0.87737 (12)	0.10107 (10)	0.15866 (8)	0.0182 (3)
H31	0.9523	0.0957	0.1882	0.022*
C32	0.76808 (13)	0.03260 (10)	0.14644 (8)	0.0185 (3)
H32	0.7676	−0.0199	0.1669	0.022*
C33	0.66014 (12)	0.04320 (10)	0.10369 (8)	0.0186 (3)
H33	0.5845	−0.0018	0.0954	0.022*
C34	0.66199 (12)	0.11944 (10)	0.07278 (8)	0.0164 (2)
H34	0.5865	0.1244	0.0437	0.020*
B2	0.21218 (12)	0.21890 (11)	0.46170 (8)	0.0132 (3)
C35	0.18977 (11)	0.10369 (10)	0.39032 (7)	0.0146 (2)
C36	0.07262 (12)	0.05578 (10)	0.33620 (8)	0.0162 (2)
H36	0.0083	0.0913	0.3421	0.019*
C37	0.04716 (13)	−0.04096 (11)	0.27466 (8)	0.0209 (3)
H37	−0.0329	−0.0695	0.2394	0.025*
C38	0.13855 (14)	−0.09602 (11)	0.26452 (9)	0.0263 (3)
H38	0.1218	−0.1622	0.2228	0.032*
C39	0.25467 (14)	−0.05202 (11)	0.31674 (9)	0.0255 (3)
H39	0.3181	−0.0886	0.3110	0.031*
C40	0.27898 (12)	0.04579 (10)	0.37778 (8)	0.0190 (3)
H40	0.3596	0.0742	0.4123	0.023*
C41	0.09474 (11)	0.21976 (9)	0.49961 (7)	0.0134 (2)
C42	0.02629 (11)	0.29574 (10)	0.50940 (8)	0.0158 (2)
H42	0.0450	0.3485	0.4906	0.019*
C43	−0.06912 (12)	0.29718 (11)	0.54603 (8)	0.0213 (3)
H43	−0.1141	0.3498	0.5510	0.026*
C44	−0.09777 (12)	0.22214 (11)	0.57497 (8)	0.0207 (3)
H44	−0.1612	0.2236	0.6007	0.025*
C45	−0.03243 (12)	0.14465 (11)	0.56592 (8)	0.0198 (3)
H45	−0.0512	0.0926	0.5854	0.024*
C46	0.06078 (12)	0.14359 (10)	0.52818 (8)	0.0176 (3)
H46	0.1031	0.0891	0.5215	0.021*
C47	0.33983 (11)	0.24479 (9)	0.53140 (7)	0.0143 (2)
C48	0.34464 (12)	0.26164 (10)	0.61014 (8)	0.0172 (3)
H48	0.2704	0.2597	0.6253	0.021*
C49	0.45487 (13)	0.28120 (11)	0.66708 (8)	0.0227 (3)
H49	0.4539	0.2924	0.7197	0.027*
C50	0.56528 (13)	0.28439 (11)	0.64765 (9)	0.0243 (3)
H50	0.6397	0.2955	0.6859	0.029*
C51	0.56484 (12)	0.27095 (10)	0.57047 (9)	0.0219 (3)
H51	0.6396	0.2738	0.5560	0.026*
C52	0.45479 (12)	0.25341 (10)	0.51484 (8)	0.0172 (3)
H52	0.4571	0.2469	0.4633	0.021*
C53	0.21969 (11)	0.31079 (10)	0.42702 (7)	0.0134 (2)
C54	0.15048 (11)	0.29751 (10)	0.35213 (7)	0.0160 (2)
H54	0.1023	0.2304	0.3175	0.019*
C55	0.14934 (12)	0.37874 (11)	0.32625 (8)	0.0183 (3)

H55	0.1013	0.3659	0.2749	0.022*
C56	0.21772 (12)	0.47772 (10)	0.37494 (8)	0.0179 (3)
H56	0.2169	0.5330	0.3575	0.021*
C57	0.28783 (12)	0.49490 (10)	0.44999 (8)	0.0183 (3)
H57	0.3352	0.5624	0.4844	0.022*
C58	0.28817 (12)	0.41266 (10)	0.47442 (8)	0.0169 (3)
H58	0.3371	0.4260	0.5256	0.020*
O1	0.34685 (13)	0.37036 (10)	0.13799 (8)	0.0436 (3)
C59	0.31258 (14)	0.44161 (12)	0.12440 (9)	0.0257 (3)
C60	0.37217 (16)	0.49196 (14)	0.07953 (11)	0.0353 (4)
H60A	0.4042	0.5662	0.1119	0.053*
H60B	0.3118	0.4827	0.0311	0.053*
H60C	0.4398	0.4601	0.0661	0.053*
C61	0.20691 (17)	0.47985 (18)	0.15014 (11)	0.0436 (5)
H61A	0.1306	0.4408	0.1088	0.065*
H61B	0.2178	0.5537	0.1599	0.065*
H61C	0.2028	0.4702	0.1986	0.065*
O2	0.59749 (11)	0.08463 (11)	0.35934 (9)	0.0449 (3)
C62	0.62729 (14)	0.00823 (11)	0.45296 (9)	0.0259 (3)
H62A	0.5788	0.0548	0.4785	0.039*
H62B	0.7044	0.0173	0.4914	0.039*
H62C	0.5808	−0.0638	0.4326	0.039*
C63	0.65441 (13)	0.03302 (11)	0.38676 (9)	0.0242 (3)
C64	0.75574 (14)	−0.00695 (13)	0.35534 (9)	0.0286 (3)
H64A	0.7550	0.0038	0.3067	0.043*
H64B	0.7439	−0.0812	0.3443	0.043*
H64C	0.8347	0.0304	0.3945	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0143 (5)	0.0173 (5)	0.0180 (5)	0.0052 (4)	0.0070 (4)	0.0075 (4)
N2	0.0124 (5)	0.0165 (5)	0.0177 (5)	0.0045 (4)	0.0041 (4)	0.0046 (4)
N3	0.0131 (5)	0.0191 (5)	0.0167 (5)	0.0029 (4)	0.0019 (4)	0.0094 (4)
C1	0.0139 (6)	0.0168 (6)	0.0105 (5)	0.0029 (5)	0.0032 (4)	0.0040 (5)
C2	0.0159 (6)	0.0206 (6)	0.0199 (6)	0.0081 (5)	0.0077 (5)	0.0070 (5)
C3	0.0214 (7)	0.0247 (7)	0.0251 (7)	0.0066 (5)	0.0110 (6)	0.0157 (6)
C4	0.0137 (6)	0.0227 (7)	0.0233 (7)	0.0003 (5)	0.0027 (5)	0.0069 (6)
C5	0.0174 (6)	0.0205 (7)	0.0302 (8)	0.0093 (5)	0.0066 (6)	0.0064 (6)
C6	0.0137 (6)	0.0203 (6)	0.0167 (6)	0.0010 (5)	0.0037 (5)	0.0082 (5)
C7	0.0149 (6)	0.0249 (7)	0.0165 (6)	0.0003 (5)	0.0031 (5)	0.0031 (5)
N4A	0.0136 (11)	0.0206 (6)	0.0163 (9)	0.0037 (5)	0.0039 (5)	0.0041 (6)
C8A	0.0192 (8)	0.0409 (14)	0.0380 (11)	0.0090 (9)	0.0061 (8)	−0.0036 (10)
C9A	0.0329 (10)	0.0352 (12)	0.0164 (8)	−0.0008 (9)	0.0011 (7)	0.0088 (8)
C10A	0.0389 (11)	0.0190 (8)	0.0346 (10)	−0.0014 (7)	0.0027 (8)	0.0101 (8)
N4B	0.0136 (11)	0.0206 (6)	0.0163 (9)	0.0037 (5)	0.0039 (5)	0.0041 (6)
C8B	0.0192 (8)	0.0409 (14)	0.0380 (11)	0.0090 (9)	0.0061 (8)	−0.0036 (10)
C9B	0.0329 (10)	0.0352 (12)	0.0164 (8)	−0.0008 (9)	0.0011 (7)	0.0088 (8)

C10B	0.0389 (11)	0.0190 (8)	0.0346 (10)	−0.0014 (7)	0.0027 (8)	0.0101 (8)
B1	0.0127 (6)	0.0164 (6)	0.0145 (6)	0.0044 (5)	0.0039 (5)	0.0082 (5)
C11	0.0124 (5)	0.0144 (6)	0.0129 (6)	0.0028 (4)	0.0023 (5)	0.0048 (5)
C12	0.0146 (6)	0.0158 (6)	0.0157 (6)	0.0039 (5)	0.0035 (5)	0.0061 (5)
C13	0.0170 (6)	0.0236 (7)	0.0174 (6)	0.0086 (5)	0.0056 (5)	0.0078 (5)
C14	0.0158 (6)	0.0245 (7)	0.0164 (6)	0.0023 (5)	0.0060 (5)	0.0063 (5)
C15	0.0210 (6)	0.0185 (6)	0.0174 (6)	0.0016 (5)	0.0069 (5)	0.0070 (5)
C16	0.0199 (6)	0.0160 (6)	0.0170 (6)	0.0049 (5)	0.0065 (5)	0.0071 (5)
C17	0.0151 (6)	0.0135 (6)	0.0177 (6)	0.0041 (5)	0.0027 (5)	0.0061 (5)
C18	0.0155 (6)	0.0179 (6)	0.0213 (6)	0.0045 (5)	0.0036 (5)	0.0087 (5)
C19	0.0151 (6)	0.0189 (6)	0.0322 (8)	0.0038 (5)	0.0026 (6)	0.0112 (6)
C20	0.0210 (7)	0.0201 (7)	0.0278 (7)	0.0030 (5)	−0.0055 (6)	0.0104 (6)
C21	0.0277 (7)	0.0239 (7)	0.0179 (7)	0.0044 (6)	−0.0009 (6)	0.0070 (6)
C22	0.0202 (6)	0.0194 (6)	0.0183 (6)	0.0054 (5)	0.0020 (5)	0.0066 (5)
C23	0.0142 (6)	0.0173 (6)	0.0143 (6)	0.0048 (5)	0.0063 (5)	0.0075 (5)
C24	0.0202 (6)	0.0192 (6)	0.0175 (6)	0.0054 (5)	0.0028 (5)	0.0064 (5)
C25	0.0242 (7)	0.0213 (7)	0.0167 (6)	0.0025 (5)	0.0026 (5)	0.0047 (5)
C26	0.0275 (7)	0.0158 (6)	0.0207 (7)	0.0033 (5)	0.0115 (6)	0.0046 (5)
C27	0.0229 (7)	0.0175 (6)	0.0254 (7)	0.0072 (5)	0.0121 (6)	0.0114 (5)
C28	0.0167 (6)	0.0181 (6)	0.0183 (6)	0.0047 (5)	0.0070 (5)	0.0094 (5)
C29	0.0139 (6)	0.0163 (6)	0.0137 (6)	0.0038 (5)	0.0053 (5)	0.0051 (5)
C30	0.0160 (6)	0.0193 (6)	0.0178 (6)	0.0044 (5)	0.0055 (5)	0.0091 (5)
C31	0.0189 (6)	0.0212 (6)	0.0159 (6)	0.0058 (5)	0.0039 (5)	0.0089 (5)
C32	0.0253 (7)	0.0158 (6)	0.0169 (6)	0.0057 (5)	0.0083 (5)	0.0077 (5)
C33	0.0192 (6)	0.0166 (6)	0.0196 (6)	0.0016 (5)	0.0088 (5)	0.0055 (5)
C34	0.0140 (6)	0.0165 (6)	0.0191 (6)	0.0044 (5)	0.0060 (5)	0.0064 (5)
B2	0.0125 (6)	0.0136 (6)	0.0139 (6)	0.0039 (5)	0.0033 (5)	0.0057 (5)
C35	0.0153 (6)	0.0154 (6)	0.0146 (6)	0.0046 (5)	0.0049 (5)	0.0070 (5)
C36	0.0157 (6)	0.0167 (6)	0.0168 (6)	0.0044 (5)	0.0047 (5)	0.0070 (5)
C37	0.0192 (6)	0.0207 (7)	0.0173 (6)	0.0007 (5)	0.0010 (5)	0.0046 (5)
C38	0.0288 (8)	0.0203 (7)	0.0215 (7)	0.0062 (6)	0.0043 (6)	−0.0004 (6)
C39	0.0249 (7)	0.0210 (7)	0.0259 (7)	0.0111 (6)	0.0071 (6)	0.0015 (6)
C40	0.0169 (6)	0.0183 (6)	0.0189 (6)	0.0055 (5)	0.0037 (5)	0.0041 (5)
C41	0.0129 (6)	0.0137 (6)	0.0115 (6)	0.0035 (4)	0.0011 (4)	0.0035 (5)
C42	0.0147 (6)	0.0157 (6)	0.0171 (6)	0.0052 (5)	0.0038 (5)	0.0063 (5)
C43	0.0176 (6)	0.0226 (7)	0.0244 (7)	0.0086 (5)	0.0081 (5)	0.0073 (6)
C44	0.0171 (6)	0.0242 (7)	0.0203 (7)	0.0043 (5)	0.0090 (5)	0.0060 (5)
C45	0.0204 (6)	0.0201 (6)	0.0203 (6)	0.0019 (5)	0.0077 (5)	0.0092 (5)
C46	0.0189 (6)	0.0170 (6)	0.0196 (6)	0.0066 (5)	0.0072 (5)	0.0083 (5)
C47	0.0149 (6)	0.0120 (5)	0.0159 (6)	0.0038 (4)	0.0029 (5)	0.0057 (5)
C48	0.0209 (6)	0.0142 (6)	0.0167 (6)	0.0045 (5)	0.0032 (5)	0.0072 (5)
C49	0.0286 (7)	0.0190 (6)	0.0173 (6)	0.0032 (5)	−0.0018 (6)	0.0087 (5)
C50	0.0209 (7)	0.0178 (6)	0.0279 (7)	0.0041 (5)	−0.0069 (6)	0.0095 (6)
C51	0.0148 (6)	0.0160 (6)	0.0310 (8)	0.0032 (5)	0.0011 (6)	0.0078 (6)
C52	0.0150 (6)	0.0160 (6)	0.0203 (6)	0.0043 (5)	0.0041 (5)	0.0070 (5)
C53	0.0115 (5)	0.0163 (6)	0.0151 (6)	0.0060 (4)	0.0058 (5)	0.0070 (5)
C54	0.0142 (6)	0.0182 (6)	0.0153 (6)	0.0044 (5)	0.0030 (5)	0.0067 (5)
C55	0.0167 (6)	0.0241 (7)	0.0170 (6)	0.0071 (5)	0.0037 (5)	0.0109 (5)

C56	0.0196 (6)	0.0199 (6)	0.0216 (7)	0.0098 (5)	0.0093 (5)	0.0130 (5)
C57	0.0225 (6)	0.0136 (6)	0.0191 (6)	0.0035 (5)	0.0064 (5)	0.0065 (5)
C58	0.0200 (6)	0.0158 (6)	0.0149 (6)	0.0038 (5)	0.0037 (5)	0.0066 (5)
O1	0.0590 (8)	0.0319 (6)	0.0381 (7)	0.0117 (6)	−0.0032 (6)	0.0205 (6)
C59	0.0257 (7)	0.0268 (7)	0.0201 (7)	0.0040 (6)	−0.0032 (6)	0.0100 (6)
C60	0.0362 (9)	0.0363 (9)	0.0447 (10)	0.0149 (7)	0.0185 (8)	0.0223 (8)
C61	0.0336 (9)	0.0724 (14)	0.0310 (9)	0.0154 (9)	0.0115 (7)	0.0248 (9)
O2	0.0324 (6)	0.0494 (8)	0.0805 (10)	0.0195 (6)	0.0191 (6)	0.0518 (8)
C62	0.0277 (7)	0.0211 (7)	0.0344 (8)	0.0084 (6)	0.0161 (6)	0.0120 (6)
C63	0.0194 (7)	0.0222 (7)	0.0351 (8)	0.0039 (5)	0.0060 (6)	0.0172 (6)
C64	0.0273 (8)	0.0392 (9)	0.0296 (8)	0.0135 (7)	0.0131 (6)	0.0204 (7)

Geometric parameters (Å, º)

N1—C1	1.3308 (16)	C25—H25	0.9500
N1—C2	1.4668 (16)	C26—C27	1.390 (2)
N1—C3	1.4674 (16)	C26—H26	0.9500
N2—C1	1.3425 (16)	C27—C28	1.3967 (19)
N2—C4	1.4609 (17)	C27—H27	0.9500
N2—C5	1.4628 (17)	C28—H28	0.9500
N3—C1	1.3508 (16)	C29—C34	1.4120 (17)
N3—C6	1.4612 (16)	C29—C30	1.4154 (18)
N3—H3	0.855 (19)	C30—C31	1.3888 (18)
C2—H2A	0.9800	C30—H30	0.9500
C2—H2B	0.9800	C31—C32	1.3955 (19)
C2—H2C	0.9800	C31—H31	0.9500
C3—H3A	0.9800	C32—C33	1.3875 (19)
C3—H3B	0.9800	C32—H32	0.9500
C3—H3C	0.9800	C33—C34	1.3945 (18)
C4—H4A	0.9800	C33—H33	0.9500
C4—H4B	0.9800	C34—H34	0.9500
C4—H4C	0.9800	B2—C41	1.6457 (18)
C5—H5A	0.9800	B2—C53	1.6478 (18)
C5—H5B	0.9800	B2—C47	1.6496 (18)
C5—H5C	0.9800	B2—C35	1.6524 (18)
C6—C7	1.5286 (18)	C35—C40	1.4001 (18)
C6—H6A	0.9900	C35—C36	1.4141 (18)
C6—H6B	0.9900	C36—C37	1.3917 (19)
C7—N4A	1.504 (5)	C36—H36	0.9500
C7—N4B	1.55 (3)	C37—C38	1.392 (2)
C7—H7A	0.9900	C37—H37	0.9500
C7—H7B	0.9900	C38—C39	1.388 (2)
N4A—C8A	1.487 (3)	C38—H38	0.9500
N4A—C10A	1.501 (3)	C39—C40	1.3989 (19)
N4A—C9A	1.504 (3)	C39—H39	0.9500
C8A—H8A1	0.9800	C40—H40	0.9500
C8A—H8A2	0.9800	C41—C42	1.3975 (17)
C8A—H8A3	0.9800	C41—C46	1.4078 (17)

C9A—H9A1	0.9800	C42—C43	1.4051 (18)
C9A—H9A2	0.9800	C42—H42	0.9500
C9A—H9A3	0.9800	C43—C44	1.385 (2)
C10A—H10A	0.9800	C43—H43	0.9500
C10A—H10B	0.9800	C44—C45	1.391 (2)
C10A—H10C	0.9800	C44—H44	0.9500
N4B—C8B	1.464 (17)	C45—C46	1.3970 (18)
N4B—C9B	1.491 (17)	C45—H45	0.9500
N4B—C10B	1.508 (17)	C46—H46	0.9500
C8B—H8B1	0.9800	C47—C48	1.4060 (18)
C8B—H8B2	0.9800	C47—C52	1.4119 (18)
C8B—H8B3	0.9800	C48—C49	1.3997 (19)
C9B—H9B1	0.9800	C48—H48	0.9500
C9B—H9B2	0.9800	C49—C50	1.385 (2)
C9B—H9B3	0.9800	C49—H49	0.9500
C10B—H10D	0.9800	C50—C51	1.398 (2)
C10B—H10E	0.9800	C50—H50	0.9500
C10B—H10F	0.9800	C51—C52	1.3916 (18)
B1—C17	1.6478 (18)	C51—H51	0.9500
B1—C11	1.6525 (18)	C52—H52	0.9500
B1—C23	1.6578 (19)	C53—C54	1.4034 (17)
B1—C29	1.6588 (18)	C53—C58	1.4088 (18)
C11—C12	1.4048 (17)	C54—C55	1.3983 (18)
C11—C16	1.4113 (17)	C54—H54	0.9500
C12—C13	1.3967 (18)	C55—C56	1.3835 (19)
C12—H12	0.9500	C55—H55	0.9500
C13—C14	1.3893 (19)	C56—C57	1.3940 (19)
C13—H13	0.9500	C56—H56	0.9500
C14—C15	1.393 (2)	C57—C58	1.3940 (18)
C14—H14	0.9500	C57—H57	0.9500
C15—C16	1.3941 (18)	C58—H58	0.9500
C15—H15	0.9500	O1—C59	1.2185 (19)
C16—H16	0.9500	C59—C60	1.488 (2)
C17—C22	1.4059 (19)	C59—C61	1.492 (2)
C17—C18	1.4124 (18)	C60—H60A	0.9800
C18—C19	1.3927 (19)	C60—H60B	0.9800
C18—H18	0.9500	C60—H60C	0.9800
C19—C20	1.392 (2)	C61—H61A	0.9800
C19—H19	0.9500	C61—H61B	0.9800
C20—C21	1.385 (2)	C61—H61C	0.9800
C20—H20	0.9500	O2—C63	1.2177 (18)
C21—C22	1.4012 (19)	C62—C63	1.488 (2)
C21—H21	0.9500	C62—H62A	0.9800
C22—H2	0.9500	C62—H62B	0.9800
C23—C28	1.4027 (18)	C62—H62C	0.9800
C23—C24	1.4058 (18)	C63—C64	1.497 (2)
C24—C25	1.3941 (19)	C64—H64A	0.9800
C24—H24	0.9500	C64—H64B	0.9800

C25—C26	1.392 (2)	C64—H64C	0.9800
C1—N1—C2	122.30 (11)	C25—C24—C23	123.20 (13)
C1—N1—C3	122.05 (11)	C25—C24—H24	118.4
C2—N1—C3	115.58 (10)	C23—C24—H24	118.4
C1—N2—C4	122.22 (11)	C26—C25—C24	120.24 (13)
C1—N2—C5	121.68 (11)	C26—C25—H25	119.9
C4—N2—C5	115.46 (11)	C24—C25—H25	119.9
C1—N3—C6	125.43 (11)	C27—C26—C25	118.37 (12)
C1—N3—H3	118.1 (12)	C27—C26—H26	120.8
C6—N3—H3	115.5 (12)	C25—C26—H26	120.8
N1—C1—N2	120.62 (11)	C26—C27—C28	120.43 (13)
N1—C1—N3	121.02 (11)	C26—C27—H27	119.8
N2—C1—N3	118.36 (12)	C28—C27—H27	119.8
N1—C2—H2A	109.5	C27—C28—C23	123.01 (12)
N1—C2—H2B	109.5	C27—C28—H28	118.5
H2A—C2—H2B	109.5	C23—C28—H28	118.5
N1—C2—H2C	109.5	C34—C29—C30	113.77 (11)
H2A—C2—H2C	109.5	C34—C29—B1	124.20 (11)
H2B—C2—H2C	109.5	C30—C29—B1	121.96 (11)
N1—C3—H3A	109.5	C31—C30—C29	123.60 (12)
N1—C3—H3B	109.5	C31—C30—H30	118.2
H3A—C3—H3B	109.5	C29—C30—H30	118.2
N1—C3—H3C	109.5	C30—C31—C32	120.34 (12)
H3A—C3—H3C	109.5	C30—C31—H31	119.8
H3B—C3—H3C	109.5	C32—C31—H31	119.8
N2—C4—H4A	109.5	C33—C32—C31	118.33 (12)
N2—C4—H4B	109.5	C33—C32—H32	120.8
H4A—C4—H4B	109.5	C31—C32—H32	120.8
N2—C4—H4C	109.5	C32—C33—C34	120.45 (12)
H4A—C4—H4C	109.5	C32—C33—H33	119.8
H4B—C4—H4C	109.5	C34—C33—H33	119.8
N2—C5—H5A	109.5	C33—C34—C29	123.50 (12)
N2—C5—H5B	109.5	C33—C34—H34	118.2
H5A—C5—H5B	109.5	C29—C34—H34	118.2
N2—C5—H5C	109.5	C41—B2—C53	108.14 (10)
H5A—C5—H5C	109.5	C41—B2—C47	109.45 (10)
H5B—C5—H5C	109.5	C53—B2—C47	108.60 (10)
N3—C6—C7	110.06 (10)	C41—B2—C35	108.30 (10)
N3—C6—H6A	109.6	C53—B2—C35	110.78 (10)
C7—C6—H6A	109.6	C47—B2—C35	111.51 (10)
N3—C6—H6B	109.6	C40—C35—C36	114.79 (11)
C7—C6—H6B	109.6	C40—C35—B2	125.26 (11)
H6A—C6—H6B	108.2	C36—C35—B2	119.95 (11)
N4A—C7—C6	114.75 (14)	C37—C36—C35	123.07 (12)
C6—C7—N4B	108.6 (6)	C37—C36—H36	118.5
N4A—C7—H7A	108.6	C35—C36—H36	118.5
C6—C7—H7A	108.6	C36—C37—C38	120.22 (12)

N4A—C7—H7B	108.6	C36—C37—H37	119.9
C6—C7—H7B	108.6	C38—C37—H37	119.9
H7A—C7—H7B	107.6	C39—C38—C37	118.52 (13)
C8A—N4A—C10A	110.4 (3)	C39—C38—H38	120.7
C8A—N4A—C7	112.2 (2)	C37—C38—H38	120.7
C10A—N4A—C7	108.6 (3)	C38—C39—C40	120.50 (13)
C8A—N4A—C9A	110.0 (3)	C38—C39—H39	119.7
C10A—N4A—C9A	107.2 (2)	C40—C39—H39	119.7
C7—N4A—C9A	108.3 (2)	C39—C40—C35	122.89 (12)
N4A—C8A—H8A1	109.5	C39—C40—H40	118.6
N4A—C8A—H8A2	109.5	C35—C40—H40	118.6
H8A1—C8A—H8A2	109.5	C42—C41—C46	115.46 (11)
N4A—C8A—H8A3	109.5	C42—C41—B2	124.15 (11)
H8A1—C8A—H8A3	109.5	C46—C41—B2	120.33 (11)
H8A2—C8A—H8A3	109.5	C41—C42—C43	122.56 (12)
N4A—C9A—H9A1	109.5	C41—C42—H42	118.7
N4A—C9A—H9A2	109.5	C43—C42—H42	118.7
H9A1—C9A—H9A2	109.5	C44—C43—C42	120.17 (12)
N4A—C9A—H9A3	109.5	C44—C43—H43	119.9
H9A1—C9A—H9A3	109.5	C42—C43—H43	119.9
H9A2—C9A—H9A3	109.5	C43—C44—C45	119.10 (12)
N4A—C10A—H10A	109.5	C43—C44—H44	120.5
N4A—C10A—H10B	109.5	C45—C44—H44	120.5
H10A—C10A—H10B	109.5	C44—C45—C46	119.87 (12)
N4A—C10A—H10C	109.5	C44—C45—H45	120.1
H10A—C10A—H10C	109.5	C46—C45—H45	120.1
H10B—C10A—H10C	109.5	C45—C46—C41	122.82 (12)
C8B—N4B—C9B	111.1 (16)	C45—C46—H46	118.6
C8B—N4B—C10B	111.3 (16)	C41—C46—H46	118.6
C9B—N4B—C10B	105.4 (14)	C48—C47—C52	115.03 (11)
C8B—N4B—C7	106.7 (14)	C48—C47—B2	124.28 (11)
C9B—N4B—C7	105.0 (13)	C52—C47—B2	120.68 (11)
C10B—N4B—C7	117.2 (15)	C49—C48—C47	122.40 (13)
N4B—C8B—H8B1	109.5	C49—C48—H48	118.8
N4B—C8B—H8B2	109.5	C47—C48—H48	118.8
H8B1—C8B—H8B2	109.5	C50—C49—C48	120.80 (13)
N4B—C8B—H8B3	109.5	C50—C49—H49	119.6
H8B1—C8B—H8B3	109.5	C48—C49—H49	119.6
H8B2—C8B—H8B3	109.5	C49—C50—C51	118.56 (12)
N4B—C9B—H9B1	109.5	C49—C50—H50	120.7
N4B—C9B—H9B2	109.5	C51—C50—H50	120.7
H9B1—C9B—H9B2	109.5	C52—C51—C50	119.99 (13)
N4B—C9B—H9B3	109.5	C52—C51—H51	120.0
H9B1—C9B—H9B3	109.5	C50—C51—H51	120.0
H9B2—C9B—H9B3	109.5	C51—C52—C47	123.11 (13)
N4B—C10B—H10D	109.5	C51—C52—H52	118.4
N4B—C10B—H10E	109.5	C47—C52—H52	118.4
H10D—C10B—H10E	109.5	C54—C53—C58	114.75 (11)

N4B—C10B—H10F	109.5	C54—C53—B2	123.50 (11)
H10D—C10B—H10F	109.5	C58—C53—B2	121.47 (11)
H10E—C10B—H10F	109.5	C55—C54—C53	122.84 (12)
C17—B1—C11	108.93 (10)	C55—C54—H54	118.6
C17—B1—C23	109.99 (10)	C53—C54—H54	118.6
C11—B1—C23	106.64 (10)	C56—C55—C54	120.43 (12)
C17—B1—C29	109.94 (10)	C56—C55—H55	119.8
C11—B1—C29	110.37 (10)	C54—C55—H55	119.8
C23—B1—C29	110.91 (10)	C55—C56—C57	118.89 (12)
C12—C11—C16	114.93 (11)	C55—C56—H56	120.6
C12—C11—B1	126.24 (11)	C57—C56—H56	120.6
C16—C11—B1	118.76 (11)	C56—C57—C58	119.72 (12)
C13—C12—C11	123.01 (12)	C56—C57—H57	120.1
C13—C12—H12	118.5	C58—C57—H57	120.1
C11—C12—H12	118.5	C57—C58—C53	123.36 (12)
C14—C13—C12	120.17 (12)	C57—C58—H58	118.3
C14—C13—H13	119.9	C53—C58—H58	118.3
C12—C13—H13	119.9	O1—C59—C60	121.36 (16)
C13—C14—C15	118.84 (12)	O1—C59—C61	121.27 (16)
C13—C14—H14	120.6	C60—C59—C61	117.35 (14)
C15—C14—H14	120.6	C59—C60—H60A	109.5
C14—C15—C16	120.11 (12)	C59—C60—H60B	109.5
C14—C15—H15	119.9	H60A—C60—H60B	109.5
C16—C15—H15	119.9	C59—C60—H60C	109.5
C15—C16—C11	122.93 (12)	H60A—C60—H60C	109.5
C15—C16—H16	118.5	H60B—C60—H60C	109.5
C11—C16—H16	118.5	C59—C61—H61A	109.5
C22—C17—C18	114.99 (12)	C59—C61—H61B	109.5
C22—C17—B1	123.53 (11)	H61A—C61—H61B	109.5
C18—C17—B1	121.48 (11)	C59—C61—H61C	109.5
C19—C18—C17	123.04 (13)	H61A—C61—H61C	109.5
C19—C18—H18	118.5	H61B—C61—H61C	109.5
C17—C18—H18	118.5	C63—C62—H62A	109.5
C20—C19—C18	120.03 (13)	C63—C62—H62B	109.5
C20—C19—H19	120.0	H62A—C62—H62B	109.5
C18—C19—H19	120.0	C63—C62—H62C	109.5
C21—C20—C19	118.94 (13)	H62A—C62—H62C	109.5
C21—C20—H20	120.5	H62B—C62—H62C	109.5
C19—C20—H20	120.5	O2—C63—C62	121.64 (14)
C20—C21—C22	120.42 (13)	O2—C63—C64	120.87 (14)
C20—C21—H21	119.8	C62—C63—C64	117.48 (12)
C22—C21—H21	119.8	C63—C64—H64A	109.5
C21—C22—C17	122.56 (13)	C63—C64—H64B	109.5
C21—C22—H2	118.7	H64A—C64—H64B	109.5
C17—C22—H2	118.7	C63—C64—H64C	109.5
C28—C23—C24	114.74 (12)	H64A—C64—H64C	109.5
C28—C23—B1	124.38 (11)	H64B—C64—H64C	109.5
C24—C23—B1	120.69 (11)		

C2—N1—C1—N2	−151.36 (12)	C23—B1—C29—C30	−73.78 (15)
C3—N1—C1—N2	31.64 (18)	C34—C29—C30—C31	1.59 (19)
C2—N1—C1—N3	29.01 (18)	B1—C29—C30—C31	−175.45 (12)
C3—N1—C1—N3	−147.99 (12)	C29—C30—C31—C32	−0.8 (2)
C4—N2—C1—N1	34.13 (18)	C30—C31—C32—C33	−0.6 (2)
C5—N2—C1—N1	−155.46 (12)	C31—C32—C33—C34	1.1 (2)
C4—N2—C1—N3	−146.24 (12)	C32—C33—C34—C29	−0.2 (2)
C5—N2—C1—N3	24.18 (18)	C30—C29—C34—C33	−1.07 (19)
C6—N3—C1—N1	35.61 (19)	B1—C29—C34—C33	175.89 (12)
C6—N3—C1—N2	−144.03 (13)	C41—B2—C35—C40	−136.36 (12)
C1—N3—C6—C7	46.52 (17)	C53—B2—C35—C40	105.20 (14)
N3—C6—C7—N4A	162.38 (16)	C47—B2—C35—C40	−15.88 (17)
N3—C6—C7—N4B	166.3 (7)	C41—B2—C35—C36	43.17 (15)
C6—C7—N4A—C8A	47.0 (3)	C53—B2—C35—C36	−75.27 (14)
C6—C7—N4A—C10A	−75.3 (2)	C47—B2—C35—C36	163.65 (11)
C6—C7—N4A—C9A	168.60 (17)	C40—C35—C36—C37	−0.51 (19)
C6—C7—N4B—C8B	80.1 (11)	B2—C35—C36—C37	179.91 (12)
C6—C7—N4B—C9B	−161.9 (9)	C35—C36—C37—C38	0.8 (2)
C6—C7—N4B—C10B	−45.3 (13)	C36—C37—C38—C39	−0.3 (2)
C17—B1—C11—C12	−107.20 (13)	C37—C38—C39—C40	−0.4 (2)
C23—B1—C11—C12	134.13 (12)	C38—C39—C40—C35	0.6 (2)
C29—B1—C11—C12	13.59 (17)	C36—C35—C40—C39	−0.18 (19)
C17—B1—C11—C16	69.79 (14)	B2—C35—C40—C39	179.37 (13)
C23—B1—C11—C16	−48.87 (14)	C53—B2—C41—C42	−8.02 (16)
C29—B1—C11—C16	−169.42 (11)	C47—B2—C41—C42	110.12 (13)
C16—C11—C12—C13	0.78 (18)	C35—B2—C41—C42	−128.12 (12)
B1—C11—C12—C13	177.87 (12)	C53—B2—C41—C46	175.05 (11)
C11—C12—C13—C14	−0.5 (2)	C47—B2—C41—C46	−66.81 (14)
C12—C13—C14—C15	−0.41 (19)	C35—B2—C41—C46	54.95 (14)
C13—C14—C15—C16	1.02 (19)	C46—C41—C42—C43	0.71 (18)
C14—C15—C16—C11	−0.7 (2)	B2—C41—C42—C43	−176.35 (12)
C12—C11—C16—C15	−0.15 (18)	C41—C42—C43—C44	0.8 (2)
B1—C11—C16—C15	−177.47 (12)	C42—C43—C44—C45	−1.2 (2)
C11—B1—C17—C22	8.33 (16)	C43—C44—C45—C46	0.1 (2)
C23—B1—C17—C22	124.87 (13)	C44—C45—C46—C41	1.4 (2)
C29—B1—C17—C22	−112.72 (13)	C42—C41—C46—C45	−1.80 (19)
C11—B1—C17—C18	−171.63 (11)	B2—C41—C46—C45	175.39 (12)
C23—B1—C17—C18	−55.09 (15)	C41—B2—C47—C48	1.73 (16)
C29—B1—C17—C18	67.32 (15)	C53—B2—C47—C48	119.59 (13)
C22—C17—C18—C19	−0.17 (19)	C35—B2—C47—C48	−118.07 (13)
B1—C17—C18—C19	179.80 (12)	C41—B2—C47—C52	−177.06 (11)
C17—C18—C19—C20	0.5 (2)	C53—B2—C47—C52	−59.21 (15)
C18—C19—C20—C21	0.0 (2)	C35—B2—C47—C52	63.13 (15)
C19—C20—C21—C22	−0.9 (2)	C52—C47—C48—C49	−2.56 (18)
C20—C21—C22—C17	1.3 (2)	B2—C47—C48—C49	178.59 (12)
C18—C17—C22—C21	−0.73 (19)	C47—C48—C49—C50	−0.2 (2)
B1—C17—C22—C21	179.31 (12)	C48—C49—C50—C51	2.0 (2)

C17—B1—C23—C28	−5.93 (16)	C49—C50—C51—C52	−0.9 (2)
C11—B1—C23—C28	112.04 (13)	C50—C51—C52—C47	−2.2 (2)
C29—B1—C23—C28	−127.76 (12)	C48—C47—C52—C51	3.77 (19)
C17—B1—C23—C24	179.36 (11)	B2—C47—C52—C51	−177.33 (12)
C11—B1—C23—C24	−62.67 (14)	C41—B2—C53—C54	−83.82 (14)
C29—B1—C23—C24	57.53 (15)	C47—B2—C53—C54	157.49 (11)
C28—C23—C24—C25	0.61 (19)	C35—B2—C53—C54	34.71 (16)
B1—C23—C24—C25	175.80 (12)	C41—B2—C53—C58	89.73 (13)
C23—C24—C25—C26	0.1 (2)	C47—B2—C53—C58	−28.96 (16)
C24—C25—C26—C27	−0.3 (2)	C35—B2—C53—C58	−151.74 (11)
C25—C26—C27—C28	−0.1 (2)	C58—C53—C54—C55	0.06 (18)
C26—C27—C28—C23	0.9 (2)	B2—C53—C54—C55	174.00 (12)
C24—C23—C28—C27	−1.07 (18)	C53—C54—C55—C56	−0.3 (2)
B1—C23—C28—C27	−176.05 (12)	C54—C55—C56—C57	0.2 (2)
C17—B1—C29—C34	−12.37 (17)	C55—C56—C57—C58	0.2 (2)
C11—B1—C29—C34	−132.55 (12)	C56—C57—C58—C53	−0.5 (2)
C23—B1—C29—C34	109.49 (13)	C54—C53—C58—C57	0.32 (19)
C17—B1—C29—C30	164.36 (11)	B2—C53—C58—C57	−173.75 (12)
C11—B1—C29—C30	44.17 (16)		

Hydrogen-bond geometry (Å, º)

Cg1, Cg2, Cg3 and Cg4 are the centroids of the C23–C28, C29–C34, C35–C40 and C53–C58 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O2	0.86 (2)	2.07 (2)	2.777 (2)	140 (2)
C9*A*—H9*A*3···O1	0.98	2.48	3.329 (2)	144
C8*B*—H8*B*1···O1	0.98	2.20	3.131 (2)	158
C7—H7*A*···O1	0.99	2.43	3.353 (2)	155
C3—H3*C*···*Cg*1	0.98	2.68	3.306 (2)	122
C9*A*—H9*A*1···*Cg*2^{i}	0.98	3.11	3.612 (2)	130
C9*B*—H9*B*2···*Cg*2^{i}	0.98	2.95	3.409 (2)	110
C10*B*—H10*E*···*Cg*3	0.98	2.48	3.337 (2)	146
C2—H2*C*···*Cg*4	0.98	2.98	3.543 (2)	118

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