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N,*N*,*N*′,*N*′,*N*″,*N*″,*N*‴,*N*‴-Octamethyl(but-2-yne)-bisamidinium bis(tetraphenylborate)

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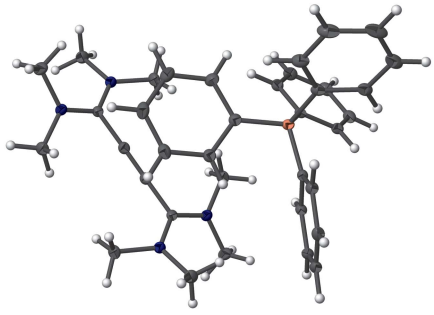
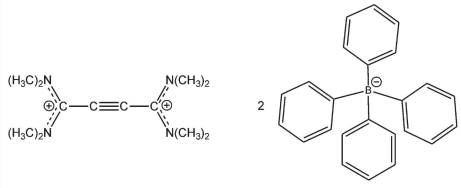
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title salt, $C_{12}H_{24}N_4^{2+}.2C_{24}H_{20}B^-$, comprises half a cation and one tetraphenylborate ion. An inversion centre is situated at the mid-point of the triple C≡C bond in the cation. The bisamidinium C—N bonds [1.3249 (11) and 1.3267 (11) Å] have double-bond character and both positive charges are delocalized between the dimethylamino groups. The bonds between the N atoms and the terminal C-methyl groups all have values characteristic for a typical single bond [1.4656 (12)–1.4687 (12) Å]. The acetylenic bond length [1.1889 (18) Å] is consistent with a triple C≡C bond and the butyne carbon chain is almost linear. C—H$\cdots\pi$ interactions between the bisamidinium methyl H atoms and the phenyl C atoms of the tetraphenylborate ions are present. The phenyl rings form aromatic pockets, in which the cations are embedded. This leads to the formation of a two-dimensional supramolecular pattern in the *ab* plane.

3D view



Chemical scheme



Structure description

Recently, we have described the preparation of *N*,*N*,*N*′,*N*′,*N*″,*N*″,*N*‴,*N*‴-octamethyl(but-2-yne)bisamidinium bis(tetrafluoroborate) by the cleavage of 1,1,1,4,4,4-hexakis(dimethylamino)-2-butyne with trifluoroacetic anhydride (Drandarov *et al.*, 2012). The salt reacts with nucleophilic reagents, yielding various amidinium and bis(amidinium) salts and ketene aminals (Drandarov *et al.*, 2015). A number of heterocyclic bis(amidinium) salts could also be prepared by cycloaddition reactions (Drandarov & Kantlehner, 2012). The title salt is the second one in our series, which has been structurally characterized after anion exchange with sodium tetraphenylborate.

The asymmetric unit contains one half of the cation and one tetraphenylborate ion. An inversion centre is situated at the mid-point of the triple C≡C bond in the cation. Prominent bond parameters in the bisamidinium ion are: N1—C1 = 1.3249 (11) Å and

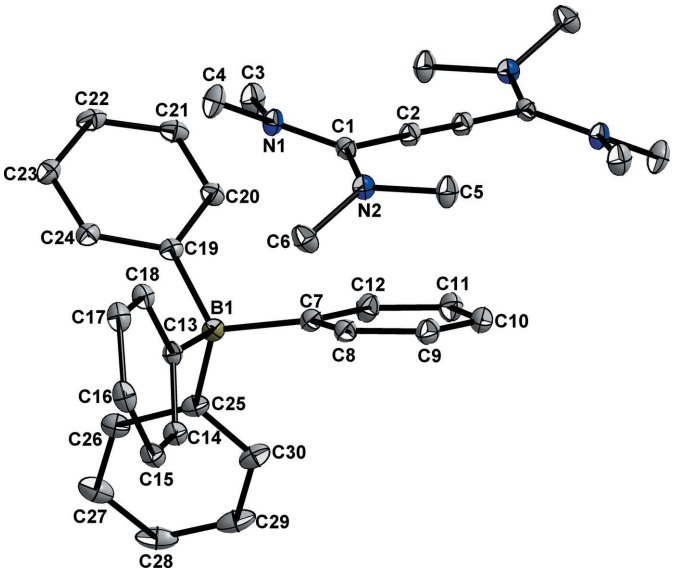


Figure 1
The structure of the title compound with displacement ellipsoids at the 50% probability level. All carbon-bonded H atoms have been omitted for clarity.

N2—C1 = 1.3267 (11) Å, indicating N—C double-bond character. Both positive charges are distributed between the dimethylamino groups. The bonds between the N atoms and the terminal *C*-methyl groups, all have values characteristic for a typical single bond [1.4656 (12)–1.4687 (12) Å]. The butyne carbon chain is almost linear, the C1—C2—C2^{i} angle being 179.0 (1)°. The C2≡C2^{i} triple bond is 1.1889 (18) Å while the C1—C2 bond length is 1.4377 (12) Å (Fig. 1).

The bond lengths of the dication agree very well with the data from the crystal structure analysis of *N*,*N*,*N*′,*N*′,-*N*″,*N*″,*N*‴,*N*‴-octamethyl(but-2-yne)bisamidinium bis(tetrafluoroborate) (Drandarov *et al.*, 2012). In the tetraphenylborate salt, the angle between the N1–C1–N2 and N1^{i}–C1^{i}–N2^{i} planes is 0° and the C1—C2—C2^{i}—C1^{i} torsion angle is 180.0 (1)°. This is completely different from the tetrafluoroborate salt (Drandarov *et al.*, 2012), where the N–C–N planes between the two amidinium units are nearly perpendicular to each other [85.1 (2)°] and C1—C2—C2^{i}—C1^{i} = 101.3 (1)°. The bond lengths and angles in the tetraphenylborate ion are in good agreement with the data for alkali metal tetraphenylborates (Behrens *et al.*, 2012).

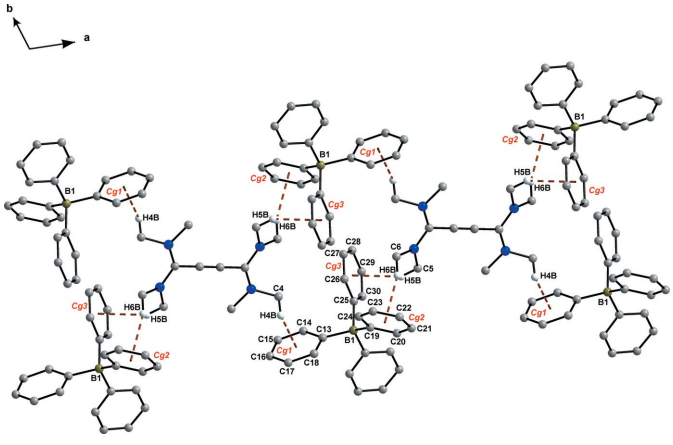


Figure 2
C—H···π interactions (brown dashed lines) between the H atoms of the bisamidinium ion and the phenyl C atoms (centroids) of the tetraphenylborate ion (*ab* view). H atoms not involved in hydrogen bonding have been omitted.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C13–C18, C19–C24 and C25–C30 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*B*···*Cg*1^{i}	0.98	2.85	3.401 (1)	116
C5—H5*B*···*Cg*3^{ii}	0.98	2.59	3.489 (1)	153
C6—H6*B*···*Cg*2^{ii}	0.98	2.54	3.487 (1)	162

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

C—H···π interactions between the hydrogen atoms of –N(CH$_3$)$_2$ groups of the cation and the phenyl carbon atoms (centroids: *Cg*1 = C13–C18, *Cg*2 = C19–C24 and *Cg*3 = C25–C30) of the tetraphenylborate ion are present (Fig. 2), ranging from 2.54 to 2.85 Å (Table 1). The phenyl rings form aromatic pockets in which the cations are embedded. This leads to the formation of a two-dimensional supramolecular pattern along the *ab* plane.

Table 2
Experimental details.

Crystal data	
Chemical formula	2(C$_{24}$H$_{20}$B)·C$_{12}$H$_{24}$N$_4$
M_r	862.77
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, *b*, *c* (Å)	13.8527 (5), 10.4892 (4), 16.7462 (6)
β (°)	103.034 (2)
V (Å^3)	2370.60 (15)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.07
Crystal size (mm)	0.35 × 0.23 × 0.10
Data collection	
Diffractometer	Bruker Kappa APEXII Duo
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	50722, 7271, 6046
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.716
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.113, 1.02
No. of reflections	7271
No. of parameters	302
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.22

Computer programs: *APEX2* (Bruker, 2008), *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg & Putz, 2005).

Synthesis and crystallization

The title compound was obtained by reacting an acetonitrile solution of *N*,*N*,*N*′,*N*′,*N*′′,*N*′′,*N*′′′,*N*′′′-octamethyl(but-2-yne)-bisamidinium bis(tetrafluoroborate) (Drandarov *et al.*, 2012*b*) with two equivalents of sodium tetraphenylborate. After stirring for one hour at room temperature, the precipitated sodium tetrafluoroborate was filtered off. The title compound crystallized from a saturated acetonitrile solution after several days at 273 K, forming yellow single crystals.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160166 [https://doi.org/10.1107/S2414314616001668]

N,*N*,*N*′,*N*′,*N*″,*N*″,*N*‴,*N*‴-Octamethyl(but-2-yne)bisamidinium bis(tetraphenylborate)

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N,*N*,*N*′,*N*′,*N*″,*N*″,*N*‴,*N*‴-Octamethylbut-2-yne)bisamidinium bis(tetraphenylborate)

Crystal data

$2(C_{24}H_{20}B)\cdot C_{12}H_{24}N_4$
M_r = 862.77
Monoclinic, $P2_1/n$
a = 13.8527 (5) Å
b = 10.4892 (4) Å
c = 16.7462 (6) Å
β = 103.034 (2)°
V = 2370.60 (15) Å^3
Z = 2
$F(000)$ = 924
D_x = 1.209 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 50722 reflections
θ = 1.7–30.6°
μ = 0.07 mm^{-1}
T = 100 K
Block, yellow
0.35 × 0.23 × 0.10 mm

Data collection

Bruker Kappa APEXII Duo diffractometer
Radiation source: fine-focus sealed tube
Triumph monochromator
φ scans, and ω scans
50722 measured reflections
7271 independent reflections
6046 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 30.6°, θ_{min} = 1.7°
h = −19→19
k = −14→14
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.113
S = 1.02
7271 reflections
302 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.7005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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. The crystal was refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.35927 (6)	0.47150 (8)	0.10360 (5)	0.01587 (15)
C1	0.36503 (6)	0.50484 (8)	0.02850 (5)	0.01380 (16)
N2	0.28770 (5)	0.54206 (8)	−0.02893 (5)	0.01533 (15)
C2	0.46046 (7)	0.50074 (9)	0.00825 (5)	0.01554 (17)
C3	0.44900 (7)	0.46323 (11)	0.16970 (6)	0.02152 (19)
H3A	0.4792	0.3789	0.1688	0.032*
H3B	0.4315	0.4763	0.2226	0.032*
H3C	0.4962	0.5290	0.1618	0.032*
C4	0.26820 (7)	0.41956 (11)	0.12146 (6)	0.0228 (2)
H4A	0.2361	0.4851	0.1482	0.034*
H4B	0.2844	0.3458	0.1579	0.034*
H4C	0.2232	0.3931	0.0702	0.034*
C5	0.29145 (7)	0.53857 (11)	−0.11567 (6)	0.02100 (19)
H5A	0.3159	0.6204	−0.1312	0.032*
H5B	0.2249	0.5228	−0.1492	0.032*
H5C	0.3361	0.4702	−0.1246	0.032*
C6	0.20340 (7)	0.60966 (10)	−0.00906 (6)	0.02072 (19)
H6A	0.1480	0.5503	−0.0124	0.031*
H6B	0.1831	0.6795	−0.0481	0.031*
H6C	0.2228	0.6444	0.0466	0.031*
B1	0.48759 (7)	0.85310 (10)	0.22798 (6)	0.01361 (17)
C7	0.51523 (7)	0.83135 (9)	0.13802 (5)	0.01530 (17)
C8	0.44148 (7)	0.82171 (9)	0.06504 (6)	0.01623 (17)
H8	0.3741	0.8182	0.0688	0.019*
C9	0.46258 (7)	0.81705 (9)	−0.01235 (6)	0.01939 (18)
H9	0.4099	0.8123	−0.0597	0.023*
C10	0.55982 (8)	0.81925 (10)	−0.02087 (6)	0.02158 (19)
H10	0.5745	0.8168	−0.0736	0.026*
C11	0.63533 (7)	0.82504 (10)	0.04943 (6)	0.0224 (2)
H11	0.7025	0.8245	0.0450	0.027*
C12	0.61303 (7)	0.83171 (10)	0.12652 (6)	0.01945 (18)
H12	0.6662	0.8367	0.1735	0.023*
C13	0.36643 (6)	0.86150 (9)	0.21106 (5)	0.01375 (16)
C14	0.31746 (7)	0.97595 (9)	0.18302 (6)	0.01610 (17)
H14	0.3559	1.0508	0.1825	0.019*
C15	0.21492 (7)	0.98402 (9)	0.15596 (6)	0.01789 (18)
H15	0.1850	1.0629	0.1363	0.021*
C16	0.15618 (7)	0.87675 (10)	0.15760 (6)	0.01854 (18)
H16	0.0862	0.8815	0.1390	0.022*

C17	0.20162 (7)	0.76264 (10)	0.18688 (6)	0.01761 (18)
H17	0.1625	0.6890	0.1895	0.021*
C18	0.30466 (6)	0.75586 (9)	0.21241 (5)	0.01508 (17)
H18	0.3341	0.6765	0.2315	0.018*
C19	0.53348 (6)	0.74262 (8)	0.29627 (5)	0.01362 (16)
C20	0.62028 (7)	0.67306 (9)	0.29618 (6)	0.01631 (17)
H20	0.6510	0.6835	0.2513	0.020*
C21	0.66342 (7)	0.58937 (9)	0.35897 (6)	0.01956 (18)
H21	0.7224	0.5451	0.3562	0.023*
C22	0.62051 (7)	0.57050 (9)	0.42547 (6)	0.02021 (19)
H22	0.6501	0.5147	0.4688	0.024*
C23	0.53331 (7)	0.63495 (9)	0.42726 (6)	0.01810 (18)
H23	0.5021	0.6221	0.4716	0.022*
C24	0.49160 (6)	0.71839 (9)	0.36407 (5)	0.01535 (17)
H24	0.4320	0.7611	0.3669	0.018*
C25	0.53179 (6)	0.99115 (9)	0.26813 (6)	0.01544 (17)
C26	0.51539 (7)	1.02990 (9)	0.34439 (6)	0.01835 (18)
H26	0.4804	0.9740	0.3725	0.022*
C27	0.54799 (8)	1.14631 (10)	0.38057 (7)	0.0242 (2)
H27	0.5351	1.1683	0.4322	0.029*
C28	0.59942 (8)	1.23028 (10)	0.34106 (8)	0.0279 (2)
H28	0.6223	1.3097	0.3654	0.034*
C29	0.61661 (8)	1.19598 (10)	0.26577 (7)	0.0267 (2)
H29	0.6518	1.2524	0.2382	0.032*
C30	0.58281 (7)	1.07926 (10)	0.22980 (6)	0.02066 (19)
H30	0.5948	1.0588	0.1776	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0133 (3)	0.0207 (4)	0.0138 (3)	0.0001 (3)	0.0034 (3)	0.0011 (3)
C1	0.0132 (4)	0.0139 (4)	0.0144 (4)	−0.0003 (3)	0.0033 (3)	−0.0013 (3)
N2	0.0130 (3)	0.0190 (4)	0.0135 (3)	0.0013 (3)	0.0022 (3)	0.0003 (3)
C2	0.0159 (4)	0.0171 (4)	0.0132 (4)	0.0009 (3)	0.0023 (3)	0.0009 (3)
C3	0.0173 (4)	0.0317 (5)	0.0141 (4)	0.0030 (4)	0.0005 (3)	0.0005 (4)
C4	0.0190 (4)	0.0307 (5)	0.0200 (4)	−0.0057 (4)	0.0073 (3)	0.0030 (4)
C5	0.0201 (4)	0.0298 (5)	0.0124 (4)	0.0000 (4)	0.0023 (3)	0.0001 (3)
C6	0.0150 (4)	0.0251 (5)	0.0212 (4)	0.0057 (3)	0.0023 (3)	−0.0021 (4)
B1	0.0117 (4)	0.0148 (4)	0.0139 (4)	−0.0003 (3)	0.0019 (3)	0.0011 (3)
C7	0.0154 (4)	0.0152 (4)	0.0154 (4)	0.0001 (3)	0.0036 (3)	0.0021 (3)
C8	0.0173 (4)	0.0158 (4)	0.0156 (4)	−0.0005 (3)	0.0036 (3)	0.0001 (3)
C9	0.0251 (5)	0.0179 (4)	0.0148 (4)	−0.0018 (3)	0.0038 (3)	−0.0002 (3)
C10	0.0297 (5)	0.0195 (4)	0.0183 (4)	−0.0013 (4)	0.0112 (4)	0.0007 (3)
C11	0.0211 (4)	0.0248 (5)	0.0241 (5)	0.0005 (4)	0.0109 (4)	0.0029 (4)
C12	0.0157 (4)	0.0240 (5)	0.0190 (4)	0.0007 (3)	0.0046 (3)	0.0033 (4)
C13	0.0132 (4)	0.0165 (4)	0.0114 (4)	0.0000 (3)	0.0024 (3)	−0.0010 (3)
C14	0.0149 (4)	0.0175 (4)	0.0155 (4)	0.0006 (3)	0.0027 (3)	−0.0001 (3)
C15	0.0164 (4)	0.0211 (4)	0.0154 (4)	0.0049 (3)	0.0017 (3)	−0.0006 (3)

C16	0.0122 (4)	0.0280 (5)	0.0148 (4)	0.0010 (3)	0.0015 (3)	−0.0038 (3)
C17	0.0137 (4)	0.0231 (5)	0.0159 (4)	−0.0035 (3)	0.0032 (3)	−0.0040 (3)
C18	0.0139 (4)	0.0170 (4)	0.0140 (4)	−0.0007 (3)	0.0022 (3)	−0.0016 (3)
C19	0.0129 (3)	0.0131 (4)	0.0138 (4)	−0.0020 (3)	0.0010 (3)	−0.0010 (3)
C20	0.0162 (4)	0.0162 (4)	0.0162 (4)	0.0002 (3)	0.0029 (3)	−0.0008 (3)
C21	0.0187 (4)	0.0165 (4)	0.0220 (4)	0.0035 (3)	0.0015 (3)	0.0006 (3)
C22	0.0236 (4)	0.0155 (4)	0.0189 (4)	0.0005 (3)	−0.0008 (3)	0.0031 (3)
C23	0.0210 (4)	0.0170 (4)	0.0157 (4)	−0.0037 (3)	0.0028 (3)	0.0015 (3)
C24	0.0145 (4)	0.0153 (4)	0.0158 (4)	−0.0018 (3)	0.0027 (3)	−0.0003 (3)
C25	0.0113 (3)	0.0154 (4)	0.0175 (4)	0.0009 (3)	−0.0011 (3)	0.0024 (3)
C26	0.0153 (4)	0.0173 (4)	0.0210 (4)	0.0007 (3)	0.0009 (3)	−0.0009 (3)
C27	0.0208 (4)	0.0198 (5)	0.0281 (5)	0.0037 (4)	−0.0027 (4)	−0.0061 (4)
C28	0.0218 (5)	0.0147 (4)	0.0408 (6)	−0.0005 (4)	−0.0066 (4)	−0.0027 (4)
C29	0.0206 (4)	0.0177 (5)	0.0377 (6)	−0.0043 (4)	−0.0018 (4)	0.0083 (4)
C30	0.0174 (4)	0.0189 (4)	0.0237 (5)	−0.0015 (3)	0.0003 (3)	0.0063 (4)

Geometric parameters (Å, º)

N1—C1	1.3249 (11)	C12—H12	0.9500
N1—C4	1.4656 (12)	C13—C18	1.4034 (12)
N1—C3	1.4687 (12)	C13—C14	1.4064 (13)
C1—N2	1.3267 (11)	C14—C15	1.3928 (12)
C1—C2	1.4377 (12)	C14—H14	0.9500
N2—C5	1.4656 (12)	C15—C16	1.3925 (14)
N2—C6	1.4672 (12)	C15—H15	0.9500
C2—C2^{i}	1.1889 (18)	C16—C17	1.3892 (14)
C3—H3A	0.9800	C16—H16	0.9500
C3—H3B	0.9800	C17—C18	1.3963 (12)
C3—H3C	0.9800	C17—H17	0.9500
C4—H4A	0.9800	C18—H18	0.9500
C4—H4B	0.9800	C19—C20	1.4068 (12)
C4—H4C	0.9800	C19—C24	1.4097 (12)
C5—H5A	0.9800	C20—C21	1.3964 (13)
C5—H5B	0.9800	C20—H20	0.9500
C5—H5C	0.9800	C21—C22	1.3897 (14)
C6—H6A	0.9800	C21—H21	0.9500
C6—H6B	0.9800	C22—C23	1.3904 (14)
C6—H6C	0.9800	C22—H22	0.9500
B1—C13	1.6404 (13)	C23—C24	1.3942 (13)
B1—C19	1.6514 (13)	C23—H23	0.9500
B1—C7	1.6517 (13)	C24—H24	0.9500
B1—C25	1.6547 (14)	C25—C30	1.4037 (13)
C7—C8	1.4086 (12)	C25—C26	1.4065 (13)
C7—C12	1.4107 (12)	C26—C27	1.3923 (14)
C8—C9	1.3923 (13)	C26—H26	0.9500
C8—H8	0.9500	C27—C28	1.3905 (17)
C9—C10	1.3863 (14)	C27—H27	0.9500
C9—H9	0.9500	C28—C29	1.3826 (18)

C10—C11	1.3886 (15)	C28—H28	0.9500
C10—H10	0.9500	C29—C30	1.3978 (15)
C11—C12	1.3953 (14)	C29—H29	0.9500
C11—H11	0.9500	C30—H30	0.9500
C1—N1—C4	122.05 (8)	C11—C12—H12	118.5
C1—N1—C3	120.61 (8)	C7—C12—H12	118.5
C4—N1—C3	116.44 (8)	C18—C13—C14	115.43 (8)
N1—C1—N2	123.66 (8)	C18—C13—B1	123.96 (8)
N1—C1—C2	118.12 (8)	C14—C13—B1	120.08 (8)
N2—C1—C2	118.22 (8)	C15—C14—C13	122.70 (9)
C1—N2—C5	120.52 (8)	C15—C14—H14	118.7
C1—N2—C6	122.11 (8)	C13—C14—H14	118.7
C5—N2—C6	116.41 (8)	C16—C15—C14	120.14 (9)
C2^{i}—C2—C1	179.01 (14)	C16—C15—H15	119.9
N1—C3—H3A	109.5	C14—C15—H15	119.9
N1—C3—H3B	109.5	C17—C16—C15	118.87 (8)
H3A—C3—H3B	109.5	C17—C16—H16	120.6
N1—C3—H3C	109.5	C15—C16—H16	120.6
H3A—C3—H3C	109.5	C16—C17—C18	120.17 (9)
H3B—C3—H3C	109.5	C16—C17—H17	119.9
N1—C4—H4A	109.5	C18—C17—H17	119.9
N1—C4—H4B	109.5	C17—C18—C13	122.66 (9)
H4A—C4—H4B	109.5	C17—C18—H18	118.7
N1—C4—H4C	109.5	C13—C18—H18	118.7
H4A—C4—H4C	109.5	C20—C19—C24	114.49 (8)
H4B—C4—H4C	109.5	C20—C19—B1	123.97 (8)
N2—C5—H5A	109.5	C24—C19—B1	121.35 (8)
N2—C5—H5B	109.5	C21—C20—C19	123.09 (9)
H5A—C5—H5B	109.5	C21—C20—H20	118.5
N2—C5—H5C	109.5	C19—C20—H20	118.5
H5A—C5—H5C	109.5	C22—C21—C20	120.35 (9)
H5B—C5—H5C	109.5	C22—C21—H21	119.8
N2—C6—H6A	109.5	C20—C21—H21	119.8
N2—C6—H6B	109.5	C21—C22—C23	118.60 (9)
H6A—C6—H6B	109.5	C21—C22—H22	120.7
N2—C6—H6C	109.5	C23—C22—H22	120.7
H6A—C6—H6C	109.5	C22—C23—C24	120.15 (9)
H6B—C6—H6C	109.5	C22—C23—H23	119.9
C13—B1—C19	112.11 (7)	C24—C23—H23	119.9
C13—B1—C7	106.77 (7)	C23—C24—C19	123.30 (8)
C19—B1—C7	113.74 (7)	C23—C24—H24	118.3
C13—B1—C25	107.07 (7)	C19—C24—H24	118.3
C19—B1—C25	106.46 (7)	C30—C25—C26	115.21 (9)
C7—B1—C25	110.54 (7)	C30—C25—B1	124.66 (8)
C8—C7—C12	114.38 (8)	C26—C25—B1	120.07 (8)
C8—C7—B1	121.95 (8)	C27—C26—C25	123.06 (10)
C12—C7—B1	123.46 (8)	C27—C26—H26	118.5

C9—C8—C7	123.14 (9)	C25—C26—H26	118.5
C9—C8—H8	118.4	C28—C27—C26	119.95 (10)
C7—C8—H8	118.4	C28—C27—H27	120.0
C10—C9—C8	120.53 (9)	C26—C27—H27	120.0
C10—C9—H9	119.7	C29—C28—C27	118.76 (10)
C8—C9—H9	119.7	C29—C28—H28	120.6
C9—C10—C11	118.50 (9)	C27—C28—H28	120.6
C9—C10—H10	120.7	C28—C29—C30	120.73 (10)
C11—C10—H10	120.7	C28—C29—H29	119.6
C10—C11—C12	120.32 (9)	C30—C29—H29	119.6
C10—C11—H11	119.8	C29—C30—C25	122.28 (10)
C12—C11—H11	119.8	C29—C30—H30	118.9
C11—C12—C7	123.09 (9)	C25—C30—H30	118.9

C4—N1—C1—N2	27.07 (14)	C15—C16—C17—C18	−1.38 (14)
C3—N1—C1—N2	−164.18 (9)	C16—C17—C18—C13	0.89 (14)
C4—N1—C1—C2	−153.09 (9)	C14—C13—C18—C17	0.72 (13)
C3—N1—C1—C2	15.67 (13)	B1—C13—C18—C17	−170.95 (8)
N1—C1—N2—C5	−160.48 (9)	C13—B1—C19—C20	149.05 (8)
C2—C1—N2—C5	19.68 (13)	C7—B1—C19—C20	27.79 (12)
N1—C1—N2—C6	31.11 (14)	C25—B1—C19—C20	−94.19 (10)
C2—C1—N2—C6	−148.73 (9)	C13—B1—C19—C24	−36.27 (11)
C13—B1—C7—C8	−0.75 (12)	C7—B1—C19—C24	−157.52 (8)
C19—B1—C7—C8	123.44 (9)	C25—B1—C19—C24	80.50 (9)
C25—B1—C7—C8	−116.87 (9)	C24—C19—C20—C21	−1.70 (13)
C13—B1—C7—C12	173.68 (8)	B1—C19—C20—C21	173.32 (9)
C19—B1—C7—C12	−62.12 (11)	C19—C20—C21—C22	0.50 (15)
C25—B1—C7—C12	57.56 (11)	C20—C21—C22—C23	1.03 (14)
C12—C7—C8—C9	−1.99 (14)	C21—C22—C23—C24	−1.24 (14)
B1—C7—C8—C9	172.92 (9)	C22—C23—C24—C19	−0.06 (14)
C7—C8—C9—C10	1.31 (15)	C20—C19—C24—C23	1.48 (13)
C8—C9—C10—C11	0.56 (15)	B1—C19—C24—C23	−173.68 (8)
C9—C10—C11—C12	−1.58 (15)	C13—B1—C25—C30	−114.00 (9)
C10—C11—C12—C7	0.83 (16)	C19—B1—C25—C30	125.92 (9)
C8—C7—C12—C11	0.92 (14)	C7—B1—C25—C30	1.93 (12)
B1—C7—C12—C11	−173.89 (9)	C13—B1—C25—C26	63.10 (10)
C19—B1—C13—C18	−34.32 (12)	C19—B1—C25—C26	−56.98 (10)
C7—B1—C13—C18	90.87 (10)	C7—B1—C25—C26	179.03 (8)
C25—B1—C13—C18	−150.71 (8)	C30—C25—C26—C27	−0.75 (13)
C19—B1—C13—C14	154.37 (8)	B1—C25—C26—C27	−178.12 (8)
C7—B1—C13—C14	−80.44 (10)	C25—C26—C27—C28	−0.03 (15)
C25—B1—C13—C14	37.98 (11)	C26—C27—C28—C29	0.36 (15)
C18—C13—C14—C15	−1.88 (13)	C27—C28—C29—C30	0.14 (15)
B1—C13—C14—C15	170.14 (8)	C28—C29—C30—C25	−1.01 (15)
C13—C14—C15—C16	1.44 (14)	C26—C25—C30—C29	1.26 (13)
C14—C15—C16—C17	0.26 (14)	B1—C25—C30—C29	178.49 (9)

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

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C13–C18, C19–C24 and C25–C30 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*B*···*Cg*1^{ii}	0.98	2.85	3.401 (1)	116
C5—H5*B*···*Cg*3^{iii}	0.98	2.59	3.489 (1)	153
C6—H6*B*···*Cg*2^{iii}	0.98	2.54	3.487 (1)	162

Symmetry codes: (ii) $-x+1/2, y-1/2, -z+1/2$; (iii) $x-1/2, -y+3/2, z-1/2$.