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4-(4-*tert*-Butylbenzyl)-1-neopentyl-1,2,4-triazolium bromide

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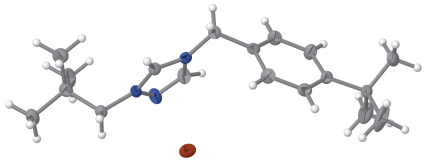
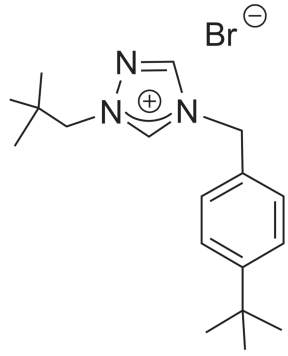
The title 1,2,4-triazolium salt, $C_{18}H_{28}N_3^+\cdot Br^-$, crystallizes in the monoclinic space group *Pc*. The extended structure exhibits a short intermolecular interaction between a heterocyclic C—H group and a bromide ion (H···Br = 2.57 Å). Additional weaker interactions exist between the other heterocyclic C—H group, an alkyl C—H group and bromide ions.

3D view



Chemical scheme



Structure description

Asymmetric 1,2,4-triazolium cations are precursors for the synthesis of *N*-heterocyclic carbenes (NHCs) and are also of interest due to their utility as cations in ionic liquids (ILs) (Dwivedi *et al.*, 2014; Nelson, 2015; Strassner *et al.*, 2013; Riederer *et al.*, 2011; Chianese *et al.*, 2004). The crystal structures of several triazolium salts have been reported (Peña Hueso *et al.*, 2022; Kumasaki *et al.*, 2021; Ponjan *et al.*, 2020; Guino-o *et al.*, 2015; Maynard *et al.*, 2023). We have synthesized many imidazolium and triazolium salts as precursors in the synthesis of NHC complexes of rhodium and iridium (Castaldi *et al.*, 2021; Gnanamgari *et al.*, 2007; Idrees *et al.*, 2017; Lerch *et al.*, 2024; Nichol *et al.*, 2011; Newman *et al.*, 2021; Rushlow *et al.*, 2022).

The molecular structure of the title complex, $C_{18}H_{28}N_3^+\cdot Br^-$, **2** (Fig. 1), consists of a triazolium cation and a bromide counter-ion. The bond lengths in the triazolium ring indicate aromaticity with C—N bonds exhibiting distances in the range of 1.292 (9)–1.368 (9) Å and an N—N bond distance of 1.376 (8) Å; the N—C—N bond angles range from 107.9 (5) to 112.1 (6)°. The bulky neopentyl and 4-tertbutyl benzyl substituents on the nitrogen atoms are in the expected *anti*-conformation with respect to the triazolium ring.

In the extended structure of **2**, several C—H···Br^- interactions are observed for heterocyclic C—H groups and an alkyl C—H group (Table 1). The non-classical hydrogen-bonding interactions are shown as dotted red lines in Fig. 2. The shortest non-

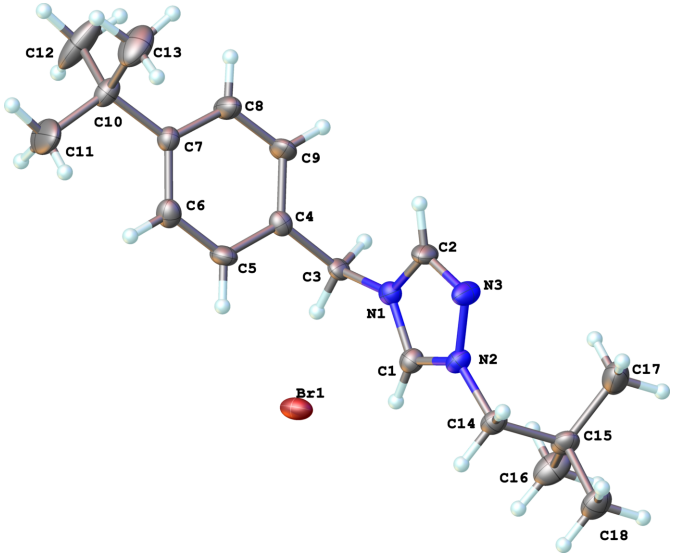


Figure 1
The molecular structure of **2** with displacement ellipsoids drawn at the 50% probability level.

standard hydrogen-bonding interaction occurs between the most acidic hydrogen atom (C1—H1) and the bromide anion.

Synthesis and crystallization

1-Neopentyl triazole (**1**) was synthesized as previously described (Mata *et al.*, 2003). All other compounds used in the syntheses as shown in Fig. 3 were obtained from Sigma-Aldrich and used as received. The synthesis was performed under nitrogen using reagent-grade solvents, which were used as received without further purification. NMR spectra were recorded at room temperature in $CDCl_3$ on a 400 MHz Varian spectrometer and referenced to the residual solvent peak (δ in p.p.m.). The title compound (**2**) crystallized as colorless needles by slow diffusion of pentane into a CH_2Cl_2 solution.

1-Meopentyl-4-(4-*tert*-butylbenzyl)-1,2,4-triazolium bromide (2): 1-neopentyl-1,2,4-triazole (**1**) (1.67 g, 11.98 mmol) and 4-*tert*-butylbenzyl bromide (5.34 g, 23.49 mmol) were added to degassed toluene (20 ml) and the mixture was refluxed in the dark for 72 h. After cooling, ether (75 ml) was added and the white solid that formed was filtered, washed with ether and air dried. Yield: 3.26 g (74%). ^{1}H NMR: $CDCl_3$, δ (p.p.m.) 11.92 (*s*, 1 H, N—C_5H—N), 8.62 (*s*, 1 H, N—C_3H—N), 7.55 (*d*, 2H, H_{arom}), 7.44 (*d*, 2H, H_{arom}), 5.84 [*s*, 2H, N—CH_2 of $CH_2C_6H_4C(CH_3)_3$], 4.28 [*s*, 2 H, CH_2 of $CH_2C(CH_3)_3$], 1.29 [*s*, 9 H, CH_3 of $C_6H_4C(CH_3)_3$], 1.04 [*s*, 9 H,

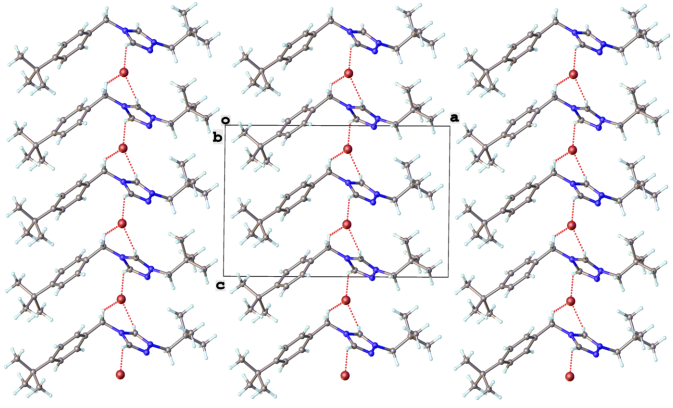


Figure 2
Crystal packing of **2** viewed along the *b*-axis direction. C—H···Br non-classical hydrogen-bonding interactions are shown as dotted red lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Br1^{i}	0.95	2.57	3.446 (6)	154
C2—H2···Br1^{ii}	0.95	2.75	3.550 (6)	143
C3—H3*B*···Br1^{iii}	0.99	2.78	3.599 (7)	141

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{28}N_3^+\cdot Br^-$
M_r	366.34
Crystal system, space group	Monoclinic, *Pc*
Temperature (K)	100
a, *b*, *c* (Å)	14.9741 (2), 6.3842 (1), 10.0741 (1)
β (°)	90.435 (1)
V (Å^3)	963.03 (2)
Z	2
Radiation type	Cu *Kα*
μ (mm^{-1})	2.90
Crystal size (mm)	0.32 × 0.06 × 0.01
Data collection	
Diffractometer	Rigaku XtaLAB Synergy-S
Absorption correction	Multi-scan [SCALE3 ABSPACK in *CrysAlis PRO* (Rigaku OD, 2024)]
T_{min}, T_{max}	0.676, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14617, 3683, 3564
R_{int}	0.067
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.043, 0.135, 1.15
No. of reflections	3683
No. of parameters	206
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.77, −0.87
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.31 (4)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

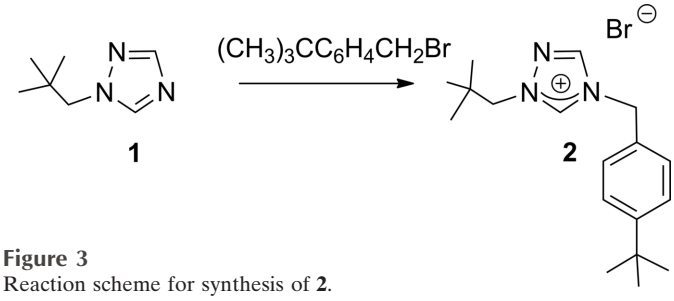


Figure 3
Reaction scheme for synthesis of **2**.

CH_3 of $CH_2C(CH_3)_3$]. ^{13}C NMR: δ 153.26 [C_{arom} of $C-C(CH_3)_3$], 143.5 ($N-C_3H-N$), 142.61 ($N-C_5H-N$), 129.09, 128.82, 126.70 (C_{arom}), 63.64 [$N-CH_2$ of $CH_2C(CH_3)_3$], 51.87 [$N-CH_2$ of $CH_2C_6H_4C(CH_3)_3$], 34.78 [C of $C_6H_4C(CH_3)_3$], 32.68 [C of $CH_2C(CH_3)_3$], 31.17 [CH_3 of $C_6H_4C(CH_3)_3$], 27.27 [CH_3 of $CH_2C(CH_3)_3$].

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. The final model was refined as an inversion twin with a Flack parameter of 0.31 (4).

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References

Castaldi, K. T., Astashkin, A. V., Albert, D. R. & Rajaseelan, E. (2021). *IUCrData*, **6**, x211142.
Chianese, A. R., Kovacevic, A., Zeglis, B. M., Faller, J. W. & Crabtree, R. H. (2004). *Organometallics*, **23**, 2461–2468.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Dwivedi, S., Gupta, S. & Das, S. (2014). *Curr. Organocatal.* (**1**), 13–39.
Gnanamgari, D., Moores, A., Rajaseelan, E. & Crabtree, R. H. (2007). *Organometallics*, **26**, 1226–1230.
Guino-o, M. A., Talbot, M. O., Slitts, M. M., Pham, T. N., Audi, M. C. & Janzen, D. E. (2015). *Acta Cryst.* E**71**, 628–635.
Idrees, K. B., Astashkin, A. V. & Rajaseelan, E. (2017). *IUCrData*, **2**, x171081.
Kumasaki, M., Gontani, S., Mori, K., Matsumoto, S. & Inoue, K. (2021). *Acta Cryst.* C**77**, 197–201.
Lerch, T. G., Gau, M., Albert, D. R. & Rajaseelan. E. (2024). *IUCrData*, **9**, x240941.
Mata, J. A., Peris, E., Incarvito, C. & Crabtree, R. H. (2003). *Chem. Commun.* pp. 184–185.
Maynard, A., Keller, T. M., Gau, M., Albert, D. R. & Rajaseelan, E. (2023). *IUCrData*, **8**, x230784.
Nelson, D. J. (2015). *Eur. J. Inorg. Chem.* pp. 2012–2027.
Newman, E. B., Astashkin, A. V., Albert, D. R. & Rajaseelan, E. (2021). *IUCrData*, **6**, x210836.
Nichol, G. S., Rajaseelan, J., Walton, D. P. & Rajaseelan, E. (2011). *Acta Cryst.* E**67**, m1860–m1861.
Peña Hueso, A., Esparza Ruiz, A. & Flores Parra, A. (2022). *IUCrData*, **7**, x220172.
Ponjan, N., Aroonchat, P. & Chainok, K. (2020). *Acta Cryst.* E**76**, 137–140.
Riederer, S. K., Bechlars, B., Herrmann, W. A. & Kühn, F. E. (2011). *Dalton Trans.* **40**, 41–43.
Rigaku OD (2024). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Rushlow, J., Astashkin, A. V., Albert, D. R. & Rajaseelan, E. (2022). *IUCrData*, **7**, x220685.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Strassner, T., Unger, Y., Meyer, D., Molt, O., Münster, I. & Wagenblast, G. (2013). *Inorg. Chem. Commun.* **30**, 39–41.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2025). **10**, x250092 [https://doi.org/10.1107/S2414314625000926]

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Crystal data

$C_{18}H_{28}N_3^+ \cdot Br^-$
M_r = 366.34
Monoclinic, *Pc*
a = 14.9741 (2) Å
b = 6.3842 (1) Å
c = 10.0741 (1) Å
β = 90.435 (1)°
V = 963.03 (2) Å^3
Z = 2
F(000) = 384
D_x = 1.263 Mg m^{-3}
Cu *K*α radiation, λ = 1.54184 Å
Cell parameters from 11602 reflections
θ = 2.9–74.4°
μ = 2.90 mm^{-1}
T = 100 K
Needle, colorless
0.32 × 0.06 × 0.01 mm

Data collection

Rigaku XtaLAB Synergy-S diffractometer
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan [SCALE3 ABSPACK in CrysAlis PRO (Rigaku OD, 2024)]
T_{min} = 0.676, T_{max} = 1.000
14617 measured reflections
3683 independent reflections
3564 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 74.5°, θ_{min} = 3.0°
h = −18→18
k = −7→6
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.135
S = 1.15
3683 reflections
206 parameters
2 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0959P)^2 + 0.2583P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.31 (4)

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. 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}
Br1	0.54656 (4)	0.06909 (7)	0.65493 (5)	0.0291 (2)
N1	0.5500 (4)	0.4637 (8)	0.3783 (5)	0.0207 (10)
N2	0.6783 (3)	0.3713 (9)	0.4539 (5)	0.0223 (9)
N3	0.6620 (4)	0.5666 (8)	0.5062 (7)	0.0274 (14)
C1	0.6101 (3)	0.3093 (10)	0.3806 (6)	0.0227 (11)
H1	0.604702	0.177837	0.337098	0.027*
C2	0.5849 (4)	0.6176 (10)	0.4576 (7)	0.0265 (12)
H2	0.555844	0.746944	0.474936	0.032*
C3	0.4647 (5)	0.4590 (10)	0.3070 (7)	0.0202 (12)
H3A	0.454105	0.316252	0.271962	0.024*
H3B	0.467148	0.556569	0.230747	0.024*
C4	0.3883 (4)	0.5206 (10)	0.3966 (6)	0.0212 (11)
C5	0.3528 (4)	0.3741 (10)	0.4850 (7)	0.0259 (11)
H5	0.378248	0.238097	0.491755	0.031*
C6	0.2802 (4)	0.4284 (9)	0.5630 (7)	0.0274 (14)
H6	0.256577	0.327384	0.622421	0.033*
C7	0.2407 (4)	0.6264 (10)	0.5570 (6)	0.0222 (10)
C8	0.2798 (4)	0.7725 (11)	0.4722 (8)	0.0307 (13)
H8	0.256487	0.910800	0.468385	0.037*
C9	0.3527 (4)	0.7196 (9)	0.3927 (7)	0.0288 (13)
H9	0.377835	0.821754	0.335496	0.035*
C10	0.1587 (4)	0.6849 (11)	0.6395 (6)	0.0271 (12)
C11	0.1228 (7)	0.5004 (18)	0.7177 (13)	0.067 (3)
H11A	0.171894	0.432843	0.766215	0.101*
H11B	0.095357	0.399365	0.656521	0.101*
H11C	0.077949	0.549817	0.780724	0.101*
C12	0.0862 (5)	0.773 (2)	0.5505 (9)	0.070 (3)
H12A	0.110278	0.890299	0.498836	0.105*
H12B	0.036538	0.823367	0.604882	0.105*
H12C	0.064673	0.663981	0.489943	0.105*
C13	0.1868 (6)	0.8531 (18)	0.7397 (10)	0.057 (2)
H13A	0.236811	0.801050	0.793659	0.085*
H13B	0.136364	0.886337	0.797395	0.085*
H13C	0.205292	0.979608	0.692129	0.085*
C14	0.7580 (4)	0.2541 (10)	0.4900 (6)	0.0252 (11)
H14A	0.742071	0.103995	0.496963	0.030*
H14B	0.778492	0.300990	0.578763	0.030*
C15	0.8356 (4)	0.2761 (11)	0.3927 (7)	0.0286 (13)
C16	0.8101 (5)	0.1791 (14)	0.2603 (8)	0.0421 (17)
H16A	0.792902	0.032522	0.273682	0.063*
H16B	0.861192	0.185658	0.200193	0.063*
H16C	0.759767	0.256349	0.221446	0.063*
C17	0.8590 (5)	0.5087 (15)	0.3764 (10)	0.0461 (18)
H17A	0.807805	0.583173	0.337805	0.069*
H17B	0.910499	0.522528	0.317528	0.069*

H17C	0.873678	0.568915	0.463317	0.069*
C18	0.9139 (4)	0.1561 (13)	0.4534 (8)	0.0374 (15)
H18A	0.928094	0.213916	0.541221	0.056*
H18B	0.966108	0.169448	0.395882	0.056*
H18C	0.897962	0.007942	0.462197	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0425 (3)	0.0204 (3)	0.0244 (3)	0.0068 (3)	0.0046 (2)	0.0019 (3)
N1	0.022 (2)	0.021 (3)	0.019 (3)	0.0001 (19)	0.002 (2)	0.0024 (19)
N2	0.019 (2)	0.026 (2)	0.021 (2)	0.005 (2)	−0.0004 (17)	0.000 (2)
N3	0.023 (3)	0.025 (3)	0.034 (3)	0.0024 (18)	−0.007 (3)	−0.011 (2)
C1	0.022 (2)	0.025 (3)	0.021 (3)	0.001 (2)	0.0011 (19)	−0.001 (2)
C2	0.026 (3)	0.017 (2)	0.037 (3)	0.002 (3)	0.000 (2)	−0.007 (3)
C3	0.021 (3)	0.016 (2)	0.024 (3)	−0.003 (2)	−0.002 (2)	−0.004 (2)
C4	0.022 (2)	0.022 (3)	0.019 (3)	−0.003 (2)	−0.003 (2)	0.000 (2)
C5	0.032 (3)	0.015 (2)	0.031 (3)	0.003 (2)	0.003 (2)	0.000 (2)
C6	0.025 (3)	0.031 (4)	0.026 (3)	−0.002 (2)	−0.001 (2)	0.006 (2)
C7	0.020 (2)	0.024 (3)	0.023 (3)	−0.001 (2)	0.0019 (19)	0.000 (2)
C8	0.032 (3)	0.025 (3)	0.036 (4)	0.007 (2)	0.010 (3)	0.008 (3)
C9	0.032 (3)	0.019 (3)	0.036 (3)	0.004 (2)	0.004 (2)	0.012 (3)
C10	0.020 (2)	0.038 (3)	0.022 (3)	0.005 (2)	0.001 (2)	−0.001 (2)
C11	0.055 (5)	0.054 (5)	0.094 (8)	0.007 (4)	0.053 (5)	0.013 (6)
C12	0.033 (3)	0.141 (10)	0.037 (4)	0.038 (5)	0.006 (3)	0.017 (5)
C13	0.041 (4)	0.076 (6)	0.053 (5)	0.003 (4)	0.013 (3)	−0.025 (5)
C14	0.023 (2)	0.027 (3)	0.025 (3)	0.006 (2)	0.000 (2)	0.003 (2)
C15	0.027 (3)	0.028 (3)	0.031 (3)	0.009 (2)	0.001 (2)	0.008 (3)
C16	0.041 (3)	0.058 (5)	0.028 (4)	0.015 (3)	−0.001 (3)	−0.006 (3)
C17	0.027 (3)	0.046 (4)	0.065 (5)	0.002 (3)	0.007 (3)	0.015 (4)
C18	0.026 (3)	0.046 (4)	0.040 (4)	0.008 (3)	−0.002 (3)	0.006 (3)

Geometric parameters (Å, º)

N1—C1	1.335 (7)	C10—C13	1.530 (11)
N1—C2	1.368 (9)	C11—H11A	0.9800
N1—C3	1.460 (8)	C11—H11B	0.9800
N2—N3	1.376 (8)	C11—H11C	0.9800
N2—C1	1.316 (8)	C12—H12A	0.9800
N2—C14	1.453 (7)	C12—H12B	0.9800
N3—C2	1.292 (9)	C12—H12C	0.9800
C1—H1	0.9500	C13—H13A	0.9800
C2—H2	0.9500	C13—H13B	0.9800
C3—H3A	0.9900	C13—H13C	0.9800
C3—H3B	0.9900	C14—H14A	0.9900
C3—C4	1.514 (9)	C14—H14B	0.9900
C4—C5	1.399 (9)	C14—C15	1.532 (8)
C4—C9	1.378 (8)	C15—C16	1.517 (11)

C5—H5	0.9500	C15—C17	1.535 (11)
C5—C6	1.391 (9)	C15—C18	1.525 (8)
C6—H6	0.9500	C16—H16A	0.9800
C6—C7	1.396 (9)	C16—H16B	0.9800
C7—C8	1.397 (9)	C16—H16C	0.9800
C7—C10	1.535 (7)	C17—H17A	0.9800
C8—H8	0.9500	C17—H17B	0.9800
C8—C9	1.400 (9)	C17—H17C	0.9800
C9—H9	0.9500	C18—H18A	0.9800
C10—C11	1.517 (12)	C18—H18B	0.9800
C10—C12	1.513 (10)	C18—H18C	0.9800

C1—N1—C2	105.4 (5)	H11A—C11—H11B	109.5
C1—N1—C3	125.5 (5)	H11A—C11—H11C	109.5
C2—N1—C3	129.1 (5)	H11B—C11—H11C	109.5
N3—N2—C14	121.3 (5)	C10—C12—H12A	109.5
C1—N2—N3	110.4 (5)	C10—C12—H12B	109.5
C1—N2—C14	128.1 (6)	C10—C12—H12C	109.5
C2—N3—N2	104.1 (5)	H12A—C12—H12B	109.5
N1—C1—H1	126.0	H12A—C12—H12C	109.5
N2—C1—N1	107.9 (5)	H12B—C12—H12C	109.5
N2—C1—H1	126.0	C10—C13—H13A	109.5
N1—C2—H2	123.9	C10—C13—H13B	109.5
N3—C2—N1	112.1 (6)	C10—C13—H13C	109.5
N3—C2—H2	123.9	H13A—C13—H13B	109.5
N1—C3—H3A	109.4	H13A—C13—H13C	109.5
N1—C3—H3B	109.4	H13B—C13—H13C	109.5
N1—C3—C4	111.3 (5)	N2—C14—H14A	108.6
H3A—C3—H3B	108.0	N2—C14—H14B	108.6
C4—C3—H3A	109.4	N2—C14—C15	114.8 (5)
C4—C3—H3B	109.4	H14A—C14—H14B	107.6
C5—C4—C3	119.9 (6)	C15—C14—H14A	108.6
C9—C4—C3	121.1 (6)	C15—C14—H14B	108.6
C9—C4—C5	119.1 (6)	C14—C15—C17	109.4 (6)
C4—C5—H5	120.2	C16—C15—C14	109.7 (6)
C6—C5—C4	119.7 (6)	C16—C15—C17	110.9 (7)
C6—C5—H5	120.2	C16—C15—C18	109.6 (6)
C5—C6—H6	118.9	C18—C15—C14	106.4 (5)
C5—C6—C7	122.3 (6)	C18—C15—C17	110.7 (6)
C7—C6—H6	118.9	C15—C16—H16A	109.5
C6—C7—C8	116.9 (5)	C15—C16—H16B	109.5
C6—C7—C10	122.5 (6)	C15—C16—H16C	109.5
C8—C7—C10	120.6 (6)	H16A—C16—H16B	109.5
C7—C8—H8	119.3	H16A—C16—H16C	109.5
C7—C8—C9	121.4 (6)	H16B—C16—H16C	109.5
C9—C8—H8	119.3	C15—C17—H17A	109.5
C4—C9—C8	120.6 (6)	C15—C17—H17B	109.5
C4—C9—H9	119.7	C15—C17—H17C	109.5

C8—C9—H9	119.7	H17A—C17—H17B	109.5
C11—C10—C7	112.3 (6)	H17A—C17—H17C	109.5
C11—C10—C13	107.4 (8)	H17B—C17—H17C	109.5
C12—C10—C7	110.1 (5)	C15—C18—H18A	109.5
C12—C10—C11	110.0 (8)	C15—C18—H18B	109.5
C12—C10—C13	108.8 (8)	C15—C18—H18C	109.5
C13—C10—C7	108.1 (5)	H18A—C18—H18B	109.5
C10—C11—H11A	109.5	H18A—C18—H18C	109.5
C10—C11—H11B	109.5	H18B—C18—H18C	109.5
C10—C11—H11C	109.5		

N1—C3—C4—C5	−79.6 (7)	C3—C4—C9—C8	177.5 (7)
N1—C3—C4—C9	100.4 (7)	C4—C5—C6—C7	−0.2 (10)
N2—N3—C2—N1	1.0 (8)	C5—C4—C9—C8	−2.5 (10)
N2—C14—C15—C16	−65.7 (7)	C5—C6—C7—C8	−2.5 (10)
N2—C14—C15—C17	56.2 (8)	C5—C6—C7—C10	178.0 (6)
N2—C14—C15—C18	175.8 (6)	C6—C7—C8—C9	2.8 (10)
N3—N2—C1—N1	2.6 (7)	C6—C7—C10—C11	−4.4 (10)
N3—N2—C14—C15	−96.1 (7)	C6—C7—C10—C12	−127.4 (8)
C1—N1—C2—N3	0.6 (8)	C6—C7—C10—C13	114.0 (8)
C1—N1—C3—C4	129.5 (6)	C7—C8—C9—C4	−0.3 (12)
C1—N2—N3—C2	−2.2 (8)	C8—C7—C10—C11	176.1 (8)
C1—N2—C14—C15	89.9 (8)	C8—C7—C10—C12	53.1 (10)
C2—N1—C1—N2	−1.9 (7)	C8—C7—C10—C13	−65.6 (8)
C2—N1—C3—C4	−48.7 (9)	C9—C4—C5—C6	2.7 (9)
C3—N1—C1—N2	179.5 (6)	C10—C7—C8—C9	−177.7 (6)
C3—N1—C2—N3	179.1 (7)	C14—N2—N3—C2	−177.2 (6)
C3—C4—C5—C6	−177.3 (6)	C14—N2—C1—N1	177.2 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Br1^{i}	0.95	2.57	3.446 (6)	154
C2—H2···Br1^{ii}	0.95	2.75	3.550 (6)	143
C3—H3*B*···Br1^{iii}	0.99	2.78	3.599 (7)	141

Symmetry codes: (i) *x*, −*y*, *z*−1/2; (ii) *x*, *y*+1, *z*; (iii) *x*, −*y*+1, *z*−1/2.