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1-Bromo-2,6-bis(4-methylpiperazin-1-ylmethyl)benzene

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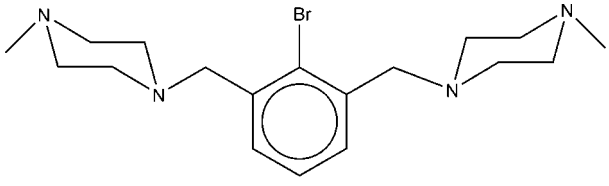
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.006 Å; R factor = 0.055; wR factor = 0.109; data-to-parameter ratio = 16.0.

In the title compound, $C_{18}H_{29}BrN_4$, both piperazine rings assume a chair conformation. Weak intermolecular C—H···Br interactions result in dimeric associations in the crystal structure. There are no further interactions between neighbouring dimer units.

Related literature

For related literature, see: Rao & Subrahmanyam (2002); Gao *et al.* (2005); Watkins *et al.* (2007); Guo (2004); Kulcsar *et al.* (2007); Velmurugan *et al.* (1994); Shanmuga Sundara Raj *et al.* (1994); Bharathi *et al.* (2006); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{18}H_{29}BrN_4$
M_r = 381.36
Triclinic, $P\overline{1}$
a = 6.0449 (5) Å
b = 12.7217 (10) Å
c = 13.6242 (11) Å
α = 68.414 (1)°
β = 81.952 (1)°
γ = 81.507 (1)°
V = 959.37 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.15 mm^{-1}
T = 297 (2) K
0.35 × 0.22 × 0.11 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.520, T_{max} = 0.798
9255 measured reflections
3359 independent reflections
2832 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.109
S = 1.17
3359 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16A···Br1^{i}	0.97	3.14	3.877 (5)	134

Symmetry code: (i) $-x+2, -y+2, -z+1$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2075).

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supplementary materials

Acta Cryst. (2007). E**63**, o4323 [**doi:10.1107/S1600536807049781**]

1-Bromo-2,6-bis(4-methylpiperazin-1-ylmethyl)benzene

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Comment

The interest in piperazine derivatives is due to their use in medicinal chemistry (Rao & Subrahmanyam, 2002; Gao *et al.*, 2005; Watkins *et al.*, 2007) and as host–guest systems (Guo, 2004). Piperazine derivatives are also important precursors for the synthesis of new hypervalent organometallic compounds containing intramolecular metal-nitrogen interactions (Kulcsar *et al.*, 2007). In order to further develop our previous work on hypervalent organoselenium derivatives containing the one pendant arm derivative, 2-[MeN(CH_2CH_2)NCH_2]C_6H_4, we synthesized the title compound and report here its crystal structure.

The molecular structure of the title compound with its atomic numbering scheme is depicted in Figure 1. The C—N bond distances [range 1.433 (5) − 1.462 (5) Å] in the piperazinyl rings are consistent with the values found in related systems (Velmurugan *et al.*, 1994; Shanmuga Sundara Raj *et al.*, 1994; Bharathi *et al.*, 2006). Both piperazinyl rings exhibit normal chair conformation with the torsion angles in the range ±56.1 (4)–58.4 (4)°.

A dimer association (Fig. 2) is formed through a soft hydrogen-bonding interaction Br···H [Br1···H16A^{i} = 3.1385 (6); C1—Br1···H16A^{i} = 115.7 (1)°; symmetry code: (i) $-x + 2, -y + 2, -z + 1$], resulting in a 12-membered ring described by the graph-set descriptor $R^2_2(9)$ (Bernstein *et al.*, 1995).

Experimental

A solution of *N*-methylpiperazine (5.83 g, 58 mmol) in benzene (100 ml) was added dropwise to a solution of 1-bromo-2,6-bis(bromomethyl)benzene (5.0 g, 14.5 mmol) in benzene (80 ml) and the reaction mixture was stirred at reflux for 8 h. After cooling to room temperature the *N*- methylpiperazinium bromide was filtered off and the solvent was evaporated at reduced pressure to give a pale yellow, viscous oil. The reaction product was purified by crystallization from a saturated hexane solution, giving the title compound as a white crystalline solid (4.0126 g, Yield: 72%). Suitable crystals for single-crystal X-ray diffraction were obtained from a warm saturated hexane solution on cooling. ^{1}H NMR ($CDCl_3$, 300 MHz): δ (p.p.m.) 2.28 (s, 6H, C*H*$_3$-N—CH_2—CH_2—N); 2.45 (br s, 8H, CH_3—N—C*H*$_2$-CH_2—N); 2.56 (br s, 8H, CH_3—N—CH_2—C*H*$_2$-N); 3.61 (s, 4H, –C*H*$_2$-C_6H_3); 7.22 (m, 1H, C_6H_3, H-4), 7.35 (d, 2H, C_6H_3, H-3,5, $^3J_{HH}$ = 7.51 Hz).^{13}C NMR ($CDCl_3$, 75.47 MHz): δ (p.p.m.) 46.06 (s, *C*H$_3$-N—CH_2—CH_2—N); 53.19 (s, CH_3—N—CH_2-*C*H_2—N); 55.2 (s, CH_3—N—C*H*$_2$-*C*H_2—N); 62.34 (s, -*C*H$_2$-C_6H_3); 126.49 (s, *C*-4); 126.70 (s, *C*-1); 128.98 (s, *C*-3,5); 138.13 (s, *C*-2,6).

Refinement

All hydrogen atoms were placed in calculated positions using a riding model, with C—H = 0.93–0.97 Å and with U_{iso}= 1.5U_{eq} (C) for methyl H and U_{iso}= 1.2U_{eq} (C) for aryl H.

Figures

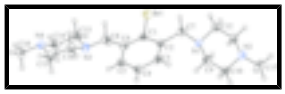

Fig. 1. : A view of the title compound showing the atom-numbering scheme at 30% probability thermal ellipsoids. H atoms are drawn as spheres of arbitrary radii.

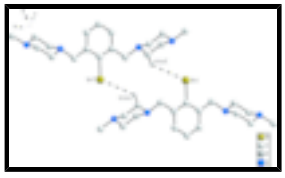

Fig. 2. : A view of the dimer formation in the title compound. H atoms not involved in hydrogen-bonding contacts have been omitted for clarity.

1-Bromo-2,6-bis(4-methylpiperazin-1-ylmethyl)benzene

Crystal data

$C_{18}H_{29}BrN_4$	$Z = 2$
$M_r = 381.36$	$F_{000} = 400$
Triclinic, $P\overline{1}$	$D_x = 1.320$ Mg m^{-3}
$a = 6.0449$ (5) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 12.7217$ (10) Å	Cell parameters from 4367 reflections
$c = 13.6242$ (11) Å	$\theta = 2.8$–26.8º
$\alpha = 68.414$ (1)º	$\mu = 2.15$ mm^{-1}
$\beta = 81.952$ (1)º	$T = 297$ (2) K
$\gamma = 81.507$ (1)º	Block, colourless
$V = 959.37$ (13) Å^3	0.35 × 0.22 × 0.11 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3359 independent reflections
Radiation source: fine-focus sealed tube	2832 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
$T = 297$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7 \rightarrow 7$
$T_{min} = 0.520$, $T_{max} = 0.798$	$k = -15 \rightarrow 15$
9255 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H-atom parameters constrained
$wR(F^2) = 0.109$	$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 0.7407P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{max} = 0.001$
3359 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
210 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.57925 (8)	0.82020 (4)	0.69557 (4)	0.06516 (19)
C1	0.6370 (6)	0.7069 (3)	0.6309 (3)	0.0417 (9)
C2	0.5553 (6)	0.6019 (3)	0.6844 (3)	0.0410 (8)
C3	0.6004 (6)	0.5231 (3)	0.6346 (3)	0.0425 (9)
H3	0.5482	0.4520	0.6678	0.051*
C4	0.7206 (6)	0.5474 (3)	0.5370 (3)	0.0435 (9)
H4	0.7490	0.4928	0.5052	0.052*
C5	0.7993 (6)	0.6520 (3)	0.4861 (3)	0.0441 (9)
H5	0.8802	0.6676	0.4199	0.053*
C6	0.7592 (6)	0.7349 (3)	0.5324 (3)	0.0419 (8)
C7	0.4353 (7)	0.5736 (3)	0.7942 (3)	0.0519 (10)
H7A	0.5420	0.5681	0.8433	0.062*
H7B	0.3207	0.6355	0.7948	0.062*
C8	0.8367 (7)	0.8515 (3)	0.4748 (3)	0.0552 (10)
H8A	0.7063	0.9059	0.4533	0.066*
H8B	0.9077	0.8725	0.5235	0.066*
C9	0.1148 (7)	0.4843 (3)	0.7882 (3)	0.0566 (10)
H9A	0.1380	0.5105	0.7115	0.068*
H9B	0.0158	0.5421	0.8080	0.068*
C10	0.0069 (7)	0.3753 (4)	0.8290 (3)	0.0564 (10)
H10A	−0.1344	0.3874	0.7984	0.068*
H10B	0.1041	0.3180	0.8078	0.068*
C11	0.1785 (6)	0.3187 (3)	0.9883 (3)	0.0524 (10)
H11A	0.2759	0.2593	0.9705	0.063*
H11B	0.1519	0.2940	1.0649	0.063*
C12	0.2939 (6)	0.4261 (3)	0.9474 (3)	0.0487 (9)

H12A	0.2025	0.4839	0.9702	0.058*
H12B	0.4373	0.4111	0.9768	0.058*
C13	1.2219 (7)	0.8154 (4)	0.4098 (3)	0.0563 (10)
H13A	1.2242	0.7365	0.4565	0.068*
H13B	1.2704	0.8581	0.4475	0.068*
C14	1.3804 (7)	0.8243 (4)	0.3124 (3)	0.0575 (11)
H14A	1.5305	0.7934	0.3329	0.069*
H14B	1.3341	0.7800	0.2756	0.069*
C15	1.1582 (7)	0.9861 (3)	0.2136 (3)	0.0559 (10)
H15A	1.1102	0.9446	0.1746	0.067*
H15B	1.1579	1.0652	0.1675	0.067*
C16	0.9951 (7)	0.9774 (3)	0.3096 (3)	0.0547 (10)
H16A	1.0370	1.0229	0.3463	0.066*
H16B	0.8455	1.0069	0.2877	0.066*
C17	−0.1452 (8)	0.2323 (4)	0.9847 (4)	0.0735 (13)
H17A	−0.0464	0.1715	0.9717	0.110*
H17B	−0.2792	0.2443	0.9499	0.110*
H17C	−0.1839	0.2129	1.0596	0.110*
C18	1.5396 (8)	0.9510 (4)	0.1482 (4)	0.0763 (14)
H18A	1.6876	0.9204	0.1692	0.114*
H18B	1.5409	1.0296	0.1037	0.114*
H18C	1.4930	0.9095	0.1097	0.114*
N1	0.3298 (5)	0.4679 (3)	0.8317 (2)	0.0444 (7)
N2	−0.0332 (5)	0.3357 (3)	0.9435 (3)	0.0510 (8)
N3	0.9942 (5)	0.8594 (2)	0.3813 (2)	0.0464 (8)
N4	1.3833 (5)	0.9412 (3)	0.2422 (2)	0.0505 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0773 (3)	0.0560 (3)	0.0734 (3)	−0.0182 (2)	0.0172 (2)	−0.0405 (2)
C1	0.040 (2)	0.042 (2)	0.051 (2)	−0.0026 (16)	−0.0053 (17)	−0.0267 (18)
C2	0.037 (2)	0.045 (2)	0.045 (2)	−0.0048 (16)	−0.0064 (16)	−0.0195 (17)
C3	0.046 (2)	0.0359 (19)	0.047 (2)	−0.0066 (16)	−0.0098 (18)	−0.0126 (17)
C4	0.046 (2)	0.040 (2)	0.050 (2)	−0.0010 (16)	−0.0089 (18)	−0.0218 (18)
C5	0.040 (2)	0.050 (2)	0.044 (2)	−0.0006 (17)	−0.0040 (17)	−0.0188 (18)
C6	0.041 (2)	0.0334 (19)	0.051 (2)	−0.0013 (16)	−0.0099 (17)	−0.0129 (17)
C7	0.055 (2)	0.055 (2)	0.051 (2)	−0.0150 (19)	0.0016 (19)	−0.024 (2)
C8	0.059 (3)	0.046 (2)	0.063 (3)	−0.0093 (19)	0.007 (2)	−0.025 (2)
C9	0.054 (3)	0.058 (3)	0.052 (2)	−0.007 (2)	−0.014 (2)	−0.009 (2)
C10	0.052 (2)	0.060 (3)	0.059 (3)	−0.010 (2)	−0.018 (2)	−0.018 (2)
C11	0.054 (2)	0.055 (2)	0.046 (2)	−0.0095 (19)	−0.0058 (19)	−0.0136 (19)
C12	0.048 (2)	0.059 (2)	0.042 (2)	−0.0106 (19)	−0.0045 (17)	−0.0201 (19)
C13	0.054 (3)	0.058 (3)	0.046 (2)	−0.005 (2)	−0.0064 (19)	−0.005 (2)
C14	0.045 (2)	0.061 (3)	0.059 (3)	0.002 (2)	−0.009 (2)	−0.013 (2)
C15	0.067 (3)	0.041 (2)	0.052 (2)	−0.007 (2)	−0.011 (2)	−0.0047 (19)
C16	0.055 (2)	0.040 (2)	0.064 (3)	−0.0036 (18)	−0.005 (2)	−0.014 (2)
C17	0.063 (3)	0.067 (3)	0.087 (3)	−0.021 (2)	−0.002 (3)	−0.020 (3)

C18	0.077 (3)	0.088 (4)	0.062 (3)	−0.025 (3)	0.012 (2)	−0.025 (3)
N1	0.0451 (18)	0.0515 (19)	0.0401 (17)	−0.0132 (15)	−0.0031 (14)	−0.0177 (15)
N2	0.0411 (18)	0.0475 (19)	0.061 (2)	−0.0094 (15)	−0.0032 (16)	−0.0135 (16)
N3	0.0443 (18)	0.0372 (17)	0.0519 (19)	−0.0045 (14)	−0.0015 (15)	−0.0100 (15)
N4	0.050 (2)	0.056 (2)	0.0449 (19)	−0.0153 (16)	0.0003 (15)	−0.0155 (16)

Geometric parameters (Å, °)

Br1—C1	1.918 (3)	C11—H11A	0.9700
C1—C6	1.386 (5)	C11—H11B	0.9700
C1—C2	1.392 (5)	C12—N1	1.461 (4)
C2—C3	1.382 (5)	C12—H12A	0.9700
C2—C7	1.507 (5)	C12—H12B	0.9700
C3—C4	1.372 (5)	C13—N3	1.456 (5)
C3—H3	0.9300	C13—C14	1.503 (5)
C4—C5	1.377 (5)	C13—H13A	0.9700
C4—H4	0.9300	C13—H13B	0.9700
C5—C6	1.392 (5)	C14—N4	1.443 (5)
C5—H5	0.9300	C14—H14A	0.9700
C6—C8	1.510 (5)	C14—H14B	0.9700
C7—N1	1.460 (5)	C15—N4	1.444 (5)
C7—H7A	0.9700	C15—C16	1.504 (5)
C7—H7B	0.9700	C15—H15A	0.9700
C8—N3	1.461 (5)	C15—H15B	0.9700
C8—H8A	0.9700	C16—N3	1.459 (4)
C8—H8B	0.9700	C16—H16A	0.9700
C9—N1	1.459 (5)	C16—H16B	0.9700
C9—C10	1.502 (5)	C17—N2	1.454 (5)
C9—H9A	0.9700	C17—H17A	0.9600
C9—H9B	0.9700	C17—H17B	0.9600
C10—N2	1.449 (5)	C17—H17C	0.9600
C10—H10A	0.9700	C18—N4	1.458 (5)
C10—H10B	0.9700	C18—H18A	0.9600
C11—N2	1.447 (5)	C18—H18B	0.9600
C11—C12	1.509 (5)	C18—H18C	0.9600
C6—C1—C2	123.6 (3)	N1—C12—H12B	109.5
C6—C1—Br1	117.5 (3)	C11—C12—H12B	109.5
C2—C1—Br1	118.9 (3)	H12A—C12—H12B	108.1
C3—C2—C1	116.8 (3)	N3—C13—C14	110.6 (3)
C3—C2—C7	121.7 (3)	N3—C13—H13A	109.5
C1—C2—C7	121.3 (3)	C14—C13—H13A	109.5
C4—C3—C2	121.4 (3)	N3—C13—H13B	109.5
C4—C3—H3	119.3	C14—C13—H13B	109.5
C2—C3—H3	119.3	H13A—C13—H13B	108.1
C3—C4—C5	120.4 (3)	N4—C14—C13	110.7 (3)
C3—C4—H4	119.8	N4—C14—H14A	109.5
C5—C4—H4	119.8	C13—C14—H14A	109.5
C4—C5—C6	120.8 (3)	N4—C14—H14B	109.5
C4—C5—H5	119.6	C13—C14—H14B	109.5

C6—C5—H5	119.6	H14A—C14—H14B	108.1
C1—C6—C5	117.0 (3)	N4—C15—C16	111.7 (3)
C1—C6—C8	122.0 (3)	N4—C15—H15A	109.3
C5—C6—C8	121.0 (3)	C16—C15—H15A	109.3
N1—C7—C2	114.0 (3)	N4—C15—H15B	109.3
N1—C7—H7A	108.7	C16—C15—H15B	109.3
C2—C7—H7A	108.7	H15A—C15—H15B	107.9
N1—C7—H7B	108.7	N3—C16—C15	110.6 (3)
C2—C7—H7B	108.7	N3—C16—H16A	109.5
H7A—C7—H7B	107.6	C15—C16—H16A	109.5
N3—C8—C6	114.0 (3)	N3—C16—H16B	109.5
N3—C8—H8A	108.7	C15—C16—H16B	109.5
C6—C8—H8A	108.7	H16A—C16—H16B	108.1
N3—C8—H8B	108.7	N2—C17—H17A	109.5
C6—C8—H8B	108.7	N2—C17—H17B	109.5
H8A—C8—H8B	107.6	H17A—C17—H17B	109.5
N1—C9—C10	110.7 (3)	N2—C17—H17C	109.5
N1—C9—H9A	109.5	H17A—C17—H17C	109.5
C10—C9—H9A	109.5	H17B—C17—H17C	109.5
N1—C9—H9B	109.5	N4—C18—H18A	109.5
C10—C9—H9B	109.5	N4—C18—H18B	109.5
H9A—C9—H9B	108.1	H18A—C18—H18B	109.5
N2—C10—C9	110.5 (3)	N4—C18—H18C	109.5
N2—C10—H10A	109.6	H18A—C18—H18C	109.5
C9—C10—H10A	109.6	H18B—C18—H18C	109.5
N2—C10—H10B	109.6	C9—N1—C7	111.4 (3)
C9—C10—H10B	109.6	C9—N1—C12	109.1 (3)
H10A—C10—H10B	108.1	C7—N1—C12	109.6 (3)
N2—C11—C12	111.6 (3)	C11—N2—C10	109.0 (3)
N2—C11—H11A	109.3	C11—N2—C17	111.3 (3)
C12—C11—H11A	109.3	C10—N2—C17	111.5 (3)
N2—C11—H11B	109.3	C13—N3—C16	108.6 (3)
C12—C11—H11B	109.3	C13—N3—C8	111.6 (3)
H11A—C11—H11B	108.0	C16—N3—C8	110.3 (3)
N1—C12—C11	110.8 (3)	C14—N4—C15	108.7 (3)
N1—C12—H12A	109.5	C14—N4—C18	111.2 (3)
C11—C12—H12A	109.5	C15—N4—C18	111.0 (3)
C6—C1—C2—C3	−0.3 (5)	N4—C15—C16—N3	−58.1 (4)
Br1—C1—C2—C3	179.8 (3)	C10—C9—N1—C7	−179.1 (3)
C6—C1—C2—C7	176.3 (3)	C10—C9—N1—C12	−57.9 (4)
Br1—C1—C2—C7	−3.6 (5)	C2—C7—N1—C9	−80.3 (4)
C1—C2—C3—C4	0.2 (5)	C2—C7—N1—C12	158.9 (3)
C7—C2—C3—C4	−176.4 (3)	C11—C12—N1—C9	56.1 (4)
C2—C3—C4—C5	−0.1 (5)	C11—C12—N1—C7	178.3 (3)
C3—C4—C5—C6	0.2 (5)	C12—C11—N2—C10	57.6 (4)
C2—C1—C6—C5	0.3 (5)	C12—C11—N2—C17	−179.0 (3)
Br1—C1—C6—C5	−179.8 (3)	C9—C10—N2—C11	−58.8 (4)
C2—C1—C6—C8	177.4 (3)	C9—C10—N2—C17	177.9 (3)
Br1—C1—C6—C8	−2.6 (5)	C14—C13—N3—C16	−58.2 (4)

C4—C5—C6—C1	−0.2 (5)	C14—C13—N3—C8	179.9 (3)
C4—C5—C6—C8	−177.4 (3)	C15—C16—N3—C13	56.9 (4)
C3—C2—C7—N1	−12.9 (5)	C15—C16—N3—C8	179.6 (3)
C1—C2—C7—N1	170.7 (3)	C6—C8—N3—C13	−80.5 (4)
C1—C6—C8—N3	170.2 (3)	C6—C8—N3—C16	158.6 (3)
C5—C6—C8—N3	−12.8 (5)	C13—C14—N4—C15	−58.5 (4)
N1—C9—C10—N2	60.2 (4)	C13—C14—N4—C18	179.1 (3)
N2—C11—C12—N1	−57.1 (4)	C16—C15—N4—C14	57.8 (4)
N3—C13—C14—N4	60.2 (4)	C16—C15—N4—C18	−179.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16A···Br1^{i}	0.97	3.14	3.877 (5)	134

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

Fig. 1

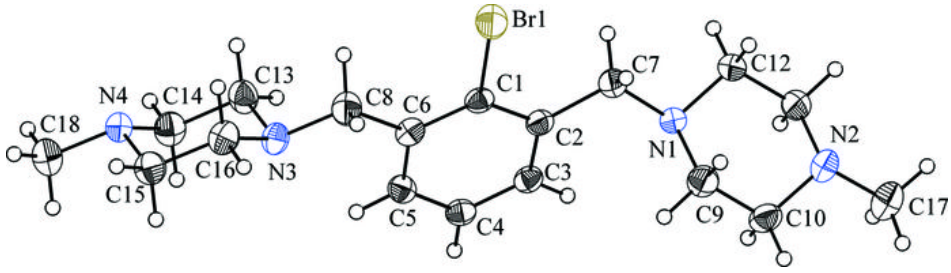
Br1
C1
C2
C3
C4
C5
C6
C7
C8
N1
C9
C10
N2
C12
C17
N3
C13
C14
C15
C16
N4
C18

Fig. 2