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## Structure Reports

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# 1-[2,2-Bis(1,3-benzimidazol-1-ylmethyl)-3-bromopropyl]-1,3-benzimidazole

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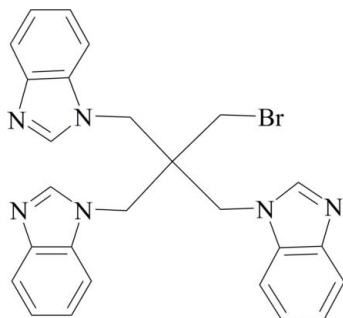
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.086; data-to-parameter ratio = 16.8.

The title compound,  $\text{C}_{26}\text{H}_{23}\text{BrN}_6$ , has been synthesized as a potential ligand for the construction of metal–organic frameworks. The three benzimidazolyl groups present three potential coordination nodes. The dihedral angles between the benzimidazole ring systems are  $74.03$  (10),  $66.49$  (9) and  $74.09$  (9)°. The structure contains large voids, which contain highly disordered solvent molecules that may be  $\text{CH}_3\text{CH}_2\text{OH}$ . Since the solvent molecules could not be located, the *PLATON/SQUEEZE* procedure [Spek (2009). *Acta Cryst. D* **65**, 148–155] was used.

## Related literature

For applications of metal organic frameworks, see: Ferey *et al.* (2005); Bradshaw *et al.* (2005); Pan *et al.* (2004); Ko *et al.* (2002); Pan *et al.* (2006); Barnett & Champness (2003); Yang *et al.* (2003); Liu *et al.* (2010). For a related structure, see: Clegg & Martin (2007).



## Experimental

## Crystal data

$\text{C}_{26}\text{H}_{23}\text{BrN}_6$	$\gamma = 84.805$ (4)°
$M_r = 499.41$	$V = 1372.9$ (10) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 2$
$a = 9.297$ (4) Å	Mo $K\alpha$ radiation
$b = 11.869$ (5) Å	$\mu = 1.52$ mm <sup>-1</sup>
$c = 13.661$ (6) Å	$T = 293$ K
$\alpha = 68.956$ (4)°	$0.32 \times 0.30 \times 0.29$ mm
$\beta = 77.398$ (4)°	

## Data collection

Bruker APEXII CCD diffractometer	9233 measured reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 2008a)	5012 independent reflections
$T_{\min} = 0.642$ , $T_{\max} = 0.667$	3417 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.025$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	299 parameters
$wR(F^2) = 0.086$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.41$ e Å <sup>-3</sup>
5012 reflections	$\Delta\rho_{\text{min}} = -0.20$ e Å <sup>-3</sup>

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008b); molecular graphics: *SHELXTL* (Sheldrick, 2008b); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2012).

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## supporting information

*Acta Cryst.* (2011). E67, o1833 [doi:10.1107/S1600536811023464]

**1-[2,2-Bis(1,3-benzimidazol-1-ylmethyl)-3-bromopropyl]-1,3-benzimidazole****Tai-Bao Wei, Yan-Yun Lu, Cheng Cao, Hong Yao and You-Ming Zhang****S1. Comment**

In recent years, metal-organic frameworks (MOFs) with network structures have received remarkable attention as a unique class of multifunctional hybrid materials with potential applications in such fields as sorption, molecular separation, luminescence, catalysis, and magnetism (Ferey *et al.*, 2005; Bradshaw *et al.*, 2005; Pan *et al.*, 2004; Ko *et al.*, 2002; Pan *et al.*, 2006). Several N-donor bridging ligands have been investigated for the construction of novel MOFs, for example 1,3-bis(4'-pyridyl)propane, 1,4-bis(4-pyridyl)butane (Barnett *et al.*, 2003), bis(2-benzimidazolymethyl)(2-pyridylmethyl)amine and bis(2-pyridylmethyl)(2-benzimidazolymethyl)amine (Yang *et al.*, 2003), 1,1'-(1,4-butanediyl)-bis[2-(2-pyridyl)benzimidazole], 1,1'-(1,6-hexanediyl)bis[2-(2-pyridyl)benzimidazole] and 1,1'-(1,1'-decane-diyl)bis-[2-(2-pyridyl)benzimidazole] (Liu *et al.*, 2010).

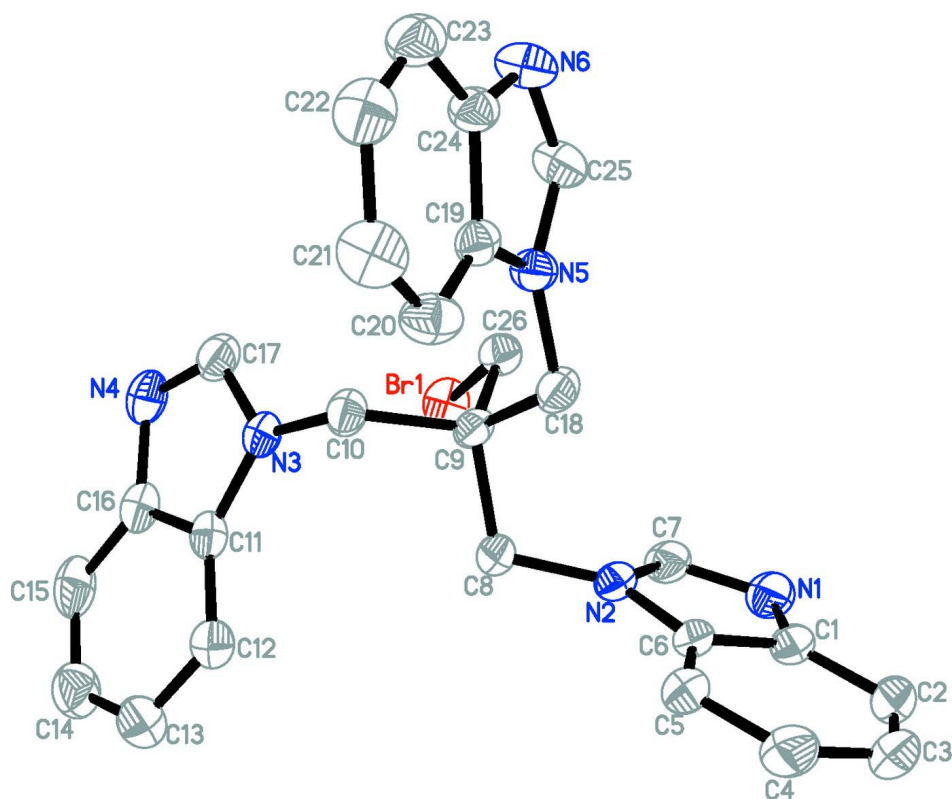
We designed and synthesized the title compound to be applied as a tridentate ligand. The molecular structure is shown in Fig. 1. This ligand is expected to be a good candidate for the construction of coordination polymers with diverse structures. First, the three benzimidazole N atoms of the ligand can act as three potential coordination nodes. Second, the three benzimidazole groups can freely twist around the quaternary carbon atom and the two  $-\text{CH}_2-$  groups to match the requirements of various coordination geometries.

**S2. Experimental**

To a solution of 1*H*-benzimidazole (30 mmol) in 100 ml of dry THF/DMSO (10:1 *v/v*) under nitrogen was added sodium hydroxide (30 mmol) with vigorous stirring at 60 °C. After 1/2 h a solution of tetrakis(bromomethyl)methane (10 mmol) in 20 ml of THF was added over a period of 1 h. The reaction mixture was stirred continuously overnight at 80 °C. A 100 ml portion of water was added to give a precipitant that was recrystallized in EtOH. Then colorless crystals suitable for X-ray diffraction analysis were grown by recrystallization from a 9:1 ethanol:water mixture (yield: 86%).

**S3. Refinement**

H atoms were included in calculated positions and refined in a riding-model approximation with C—H distances ranging from 0.93 Å to 0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ . The structure contains large voids, but the disordered solvent molecules could not be located from difference Fourier maps. The PLATON/SQUEEZE procedure (Spek, 2009) was used to account for the electron density in this region.

**Figure 1**

The structure of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

### 1-[2,2-Bis(1,3-benzimidazol-1-ylmethyl)-3-bromopropyl]-1,3-benzimidazole

#### Crystal data

$C_{26}H_{23}BrN_6$

$M_r = 499.41$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 9.297(4) \text{ \AA}$

$b = 11.869(5) \text{ \AA}$

$c = 13.661(6) \text{ \AA}$

$\alpha = 68.956(4)^\circ$

$\beta = 77.398(4)^\circ$

$\gamma = 84.805(4)^\circ$

$V = 1372.9(10) \text{ \AA}^3$

$Z = 2$

$F(000) = 512$

$D_x = 1.208 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2851 reflections

$\theta = 2.2\text{--}22.5^\circ$

$\mu = 1.52 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

$0.32 \times 0.30 \times 0.29 \text{ mm}$

#### Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 2008a)

$T_{\min} = 0.642$ ,  $T_{\max} = 0.667$

9233 measured reflections

5012 independent reflections

3417 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 25.5^\circ$ ,  $\theta_{\min} = 2.2^\circ$

$h = -10 \rightarrow 11$

$k = -14 \rightarrow 14$

$l = -12 \rightarrow 16$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.086$   
 $S = 1.01$   
 5012 reflections  
 299 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  
 $w = 1/[\sigma^2(F_o^2) + (0.040P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.41 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.20 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: *SHELXL97* (Sheldrick,  
 2008a),  $F_c^* = kFc[1 + 0.001xFc^2/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0027 (7)

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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.02589 (3)	0.37659 (2)	0.17904 (2)	0.05951 (14)
C18	0.1102 (3)	0.7601 (2)	0.0752 (2)	0.0474 (7)
H18A	0.1910	0.8026	0.0803	0.057*
H18B	0.1263	0.7613	0.0023	0.057*
C9	0.1151 (3)	0.6271 (2)	0.15110 (19)	0.0398 (6)
C26	0.0088 (3)	0.5573 (2)	0.1246 (2)	0.0475 (7)
H26A	0.0211	0.5846	0.0473	0.057*
H26B	-0.0907	0.5791	0.1523	0.057*
C10	0.0700 (3)	0.6261 (2)	0.26770 (19)	0.0463 (6)
H10A	0.1418	0.6722	0.2791	0.056*
H10B	-0.0242	0.6680	0.2748	0.056*
C8	0.2758 (3)	0.5812 (2)	0.13182 (18)	0.0430 (6)
H8A	0.3360	0.6227	0.1576	0.052*
H8B	0.2794	0.4958	0.1735	0.052*
C2	0.5675 (3)	0.7424 (3)	-0.2327 (2)	0.0725 (10)
H2	0.5874	0.7320	-0.2987	0.087*
C5	0.5050 (3)	0.7772 (3)	-0.0330 (2)	0.0596 (8)
H5	0.4843	0.7890	0.0324	0.072*
C1	0.4692 (3)	0.6679 (3)	-0.1461 (2)	0.0540 (7)
C6	0.4383 (3)	0.6874 (2)	-0.0490 (2)	0.0449 (6)
N2	0.3398 (2)	0.59903 (18)	0.01862 (16)	0.0443 (5)
C3	0.6335 (4)	0.8309 (4)	-0.2175 (3)	0.0846 (11)
H3	0.7004	0.8812	-0.2739	0.101*

N1	0.3930 (3)	0.5689 (2)	-0.1371 (2)	0.0638 (7)
C7	0.3198 (3)	0.5320 (3)	-0.0377 (2)	0.0541 (7)
H7	0.2592	0.4650	-0.0088	0.065*
N5	-0.0269 (2)	0.82613 (18)	0.09621 (16)	0.0451 (5)
C21	-0.0100 (4)	1.0452 (3)	0.2290 (3)	0.0700 (9)
H21	0.0508	1.0786	0.2568	0.084*
C19	-0.0459 (3)	0.9106 (2)	0.14554 (19)	0.0411 (6)
C24	-0.1927 (3)	0.9483 (2)	0.1476 (2)	0.0473 (7)
C20	0.0481 (3)	0.9582 (2)	0.1851 (2)	0.0574 (8)
H20	0.1461	0.9332	0.1826	0.069*
C22	-0.1552 (4)	1.0840 (2)	0.2327 (2)	0.0658 (8)
H22	-0.1899	1.1435	0.2618	0.079*
C25	-0.1577 (3)	0.8192 (2)	0.0705 (2)	0.0570 (7)
H25	-0.1722	0.7694	0.0343	0.068*
N6	-0.2618 (3)	0.8885 (2)	0.1011 (2)	0.0629 (7)
C23	-0.2491 (3)	1.0351 (2)	0.1936 (2)	0.0609 (8)
H23	-0.3476	1.0594	0.1977	0.073*
N3	0.0574 (2)	0.50904 (18)	0.35181 (15)	0.0449 (5)
C15	0.1751 (4)	0.2541 (3)	0.5510 (2)	0.0690 (9)
H15	0.1316	0.1831	0.6008	0.083*
C11	0.1656 (3)	0.4432 (2)	0.40562 (19)	0.0449 (6)
C14	0.3172 (4)	0.2784 (3)	0.5444 (3)	0.0776 (10)
H14	0.3712	0.2230	0.5908	0.093*
N4	-0.0525 (3)	0.3426 (2)	0.47523 (18)	0.0602 (6)
C17	-0.0684 (3)	0.4455 (3)	0.3981 (2)	0.0558 (7)
H17	-0.1580	0.4720	0.3774	0.067*
C16	0.0956 (3)	0.3389 (2)	0.4807 (2)	0.0524 (7)
C13	0.3842 (4)	0.3829 (3)	0.4708 (3)	0.0735 (9)
H13	0.4817	0.3964	0.4695	0.088*
C12	0.3103 (3)	0.4681 (3)	0.3990 (2)	0.0558 (7)
H12	0.3556	0.5381	0.3490	0.067*
C4	0.6031 (3)	0.8479 (3)	-0.1189 (3)	0.0792 (10)
H4	0.6508	0.9090	-0.1113	0.095*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.0688 (2)	0.05000 (18)	0.0600 (2)	-0.00572 (13)	-0.00812 (15)	-0.02107 (14)
C18	0.0433 (16)	0.0465 (14)	0.0429 (15)	0.0003 (12)	0.0019 (12)	-0.0106 (12)
C9	0.0348 (14)	0.0419 (13)	0.0385 (14)	-0.0003 (11)	0.0007 (11)	-0.0138 (12)
C26	0.0453 (15)	0.0486 (15)	0.0469 (16)	0.0027 (12)	-0.0081 (13)	-0.0160 (13)
C10	0.0509 (16)	0.0438 (14)	0.0379 (15)	0.0012 (12)	-0.0021 (12)	-0.0110 (12)
C8	0.0403 (15)	0.0491 (14)	0.0373 (15)	0.0027 (12)	-0.0040 (12)	-0.0151 (12)
C2	0.0505 (19)	0.103 (3)	0.0463 (19)	0.0172 (19)	-0.0022 (16)	-0.0139 (19)
C5	0.0447 (17)	0.076 (2)	0.0490 (18)	-0.0088 (15)	-0.0048 (14)	-0.0120 (16)
C1	0.0388 (16)	0.0732 (19)	0.0470 (18)	0.0132 (14)	-0.0046 (13)	-0.0229 (16)
C6	0.0312 (14)	0.0562 (16)	0.0407 (16)	0.0026 (12)	-0.0033 (12)	-0.0120 (13)
N2	0.0353 (12)	0.0538 (13)	0.0438 (13)	0.0039 (10)	-0.0035 (10)	-0.0208 (11)

C3	0.047 (2)	0.111 (3)	0.064 (2)	-0.0079 (19)	0.0009 (17)	0.002 (2)
N1	0.0553 (15)	0.0879 (19)	0.0571 (16)	0.0131 (14)	-0.0085 (13)	-0.0406 (15)
C7	0.0444 (17)	0.0694 (18)	0.0553 (19)	0.0089 (14)	-0.0068 (15)	-0.0341 (16)
N5	0.0389 (13)	0.0449 (12)	0.0477 (13)	0.0017 (10)	-0.0091 (10)	-0.0117 (11)
C21	0.077 (2)	0.0537 (18)	0.087 (2)	-0.0039 (17)	-0.0230 (19)	-0.0290 (18)
C19	0.0403 (15)	0.0350 (13)	0.0406 (15)	-0.0025 (11)	-0.0032 (12)	-0.0068 (12)
C24	0.0426 (16)	0.0414 (14)	0.0509 (16)	0.0054 (12)	-0.0074 (13)	-0.0101 (13)
C20	0.0459 (17)	0.0478 (16)	0.074 (2)	-0.0052 (13)	-0.0127 (15)	-0.0149 (15)
C22	0.079 (2)	0.0481 (17)	0.069 (2)	0.0018 (16)	-0.0088 (18)	-0.0223 (16)
C25	0.0565 (19)	0.0576 (17)	0.0657 (19)	0.0096 (15)	-0.0276 (16)	-0.0254 (15)
N6	0.0518 (15)	0.0614 (15)	0.0823 (18)	0.0124 (12)	-0.0266 (13)	-0.0287 (14)
C23	0.0544 (18)	0.0502 (16)	0.0648 (19)	0.0089 (14)	-0.0052 (15)	-0.0104 (15)
N3	0.0456 (13)	0.0468 (12)	0.0356 (12)	-0.0061 (10)	0.0002 (10)	-0.0100 (10)
C15	0.098 (3)	0.0493 (17)	0.0428 (18)	0.0025 (18)	-0.0012 (18)	-0.0049 (14)
C11	0.0558 (18)	0.0424 (14)	0.0349 (15)	-0.0002 (13)	-0.0059 (13)	-0.0135 (12)
C14	0.087 (3)	0.076 (2)	0.059 (2)	0.016 (2)	-0.018 (2)	-0.0117 (19)
N4	0.0685 (18)	0.0572 (15)	0.0433 (14)	-0.0157 (12)	0.0054 (12)	-0.0100 (12)
C17	0.0486 (17)	0.0661 (19)	0.0484 (17)	-0.0073 (14)	0.0019 (14)	-0.0198 (16)
C16	0.063 (2)	0.0474 (16)	0.0401 (16)	-0.0034 (14)	0.0019 (14)	-0.0144 (14)
C13	0.070 (2)	0.092 (2)	0.063 (2)	0.0081 (19)	-0.0207 (18)	-0.030 (2)
C12	0.0565 (19)	0.0617 (17)	0.0452 (17)	0.0004 (14)	-0.0085 (14)	-0.0150 (14)
C4	0.052 (2)	0.090 (2)	0.079 (3)	-0.0160 (17)	-0.0116 (18)	-0.008 (2)

*Geometric parameters (Å, °)*

Br1—C26	2.005 (3)	N5—C19	1.375 (3)
C18—N5	1.463 (3)	C21—C22	1.383 (4)
C18—C9	1.550 (3)	C21—C20	1.384 (4)
C18—H18A	0.9700	C21—H21	0.9300
C18—H18B	0.9700	C19—C20	1.375 (4)
C9—C26	1.522 (3)	C19—C24	1.395 (3)
C9—C8	1.543 (3)	C24—N6	1.381 (3)
C9—C10	1.552 (3)	C24—C23	1.398 (4)
C26—H26A	0.9700	C20—H20	0.9300
C26—H26B	0.9700	C22—C23	1.379 (4)
C10—N3	1.445 (3)	C22—H22	0.9300
C10—H10A	0.9700	C25—N6	1.310 (3)
C10—H10B	0.9700	C25—H25	0.9300
C8—N2	1.475 (3)	C23—H23	0.9300
C8—H8A	0.9700	N3—C17	1.354 (3)
C8—H8B	0.9700	N3—C11	1.389 (3)
C2—C3	1.362 (5)	C15—C14	1.354 (4)
C2—C1	1.393 (4)	C15—C16	1.401 (4)
C2—H2	0.9300	C15—H15	0.9300
C5—C4	1.370 (4)	C11—C12	1.380 (4)
C5—C6	1.383 (4)	C11—C16	1.397 (3)
C5—H5	0.9300	C14—C13	1.382 (4)
C1—N1	1.381 (4)	C14—H14	0.9300

C1—C6	1.393 (4)	N4—C17	1.316 (3)
C6—N2	1.379 (3)	N4—C16	1.391 (4)
N2—C7	1.337 (3)	C17—H17	0.9300
C3—C4	1.397 (5)	C13—C12	1.383 (4)
C3—H3	0.9300	C13—H13	0.9300
N1—C7	1.313 (3)	C12—H12	0.9300
C7—H7	0.9300	C4—H4	0.9300
N5—C25	1.354 (3)		
N5—C18—C9	115.32 (19)	C25—N5—C18	128.1 (2)
N5—C18—H18A	108.4	C19—N5—C18	125.5 (2)
C9—C18—H18A	108.4	C22—C21—C20	122.2 (3)
N5—C18—H18B	108.4	C22—C21—H21	118.9
C9—C18—H18B	108.4	C20—C21—H21	118.9
H18A—C18—H18B	107.5	C20—C19—N5	132.8 (2)
C26—C9—C8	112.7 (2)	C20—C19—C24	122.2 (2)
C26—C9—C18	107.1 (2)	N5—C19—C24	105.0 (2)
C8—C9—C18	107.56 (18)	N6—C24—C19	110.6 (2)
C26—C9—C10	112.5 (2)	N6—C24—C23	129.6 (3)
C8—C9—C10	109.21 (19)	C19—C24—C23	119.8 (3)
C18—C9—C10	107.49 (19)	C19—C20—C21	116.9 (3)
C9—C26—Br1	117.62 (17)	C19—C20—H20	121.5
C9—C26—H26A	107.9	C21—C20—H20	121.5
Br1—C26—H26A	107.9	C23—C22—C21	120.5 (3)
C9—C26—H26B	107.9	C23—C22—H22	119.7
Br1—C26—H26B	107.9	C21—C22—H22	119.7
H26A—C26—H26B	107.2	N6—C25—N5	114.2 (3)
N3—C10—C9	116.5 (2)	N6—C25—H25	122.9
N3—C10—H10A	108.2	N5—C25—H25	122.9
C9—C10—H10A	108.2	C25—N6—C24	103.8 (2)
N3—C10—H10B	108.2	C22—C23—C24	118.4 (3)
C9—C10—H10B	108.2	C22—C23—H23	120.8
H10A—C10—H10B	107.3	C24—C23—H23	120.8
N2—C8—C9	113.94 (19)	C17—N3—C11	106.5 (2)
N2—C8—H8A	108.8	C17—N3—C10	125.3 (2)
C9—C8—H8A	108.8	C11—N3—C10	128.1 (2)
N2—C8—H8B	108.8	C14—C15—C16	118.0 (3)
C9—C8—H8B	108.8	C14—C15—H15	121.0
H8A—C8—H8B	107.7	C16—C15—H15	121.0
C3—C2—C1	117.7 (3)	C12—C11—N3	132.1 (2)
C3—C2—H2	121.1	C12—C11—C16	122.6 (2)
C1—C2—H2	121.1	N3—C11—C16	105.1 (2)
C4—C5—C6	116.3 (3)	C15—C14—C13	121.9 (3)
C4—C5—H5	121.8	C15—C14—H14	119.0
C6—C5—H5	121.8	C13—C14—H14	119.0
N1—C1—C6	109.9 (2)	C17—N4—C16	104.3 (2)
N1—C1—C2	130.2 (3)	N4—C17—N3	113.9 (3)
C6—C1—C2	120.0 (3)	N4—C17—H17	123.0

N2—C6—C5	132.1 (3)	N3—C17—H17	123.0
N2—C6—C1	105.3 (2)	N4—C16—C11	110.1 (2)
C5—C6—C1	122.5 (3)	N4—C16—C15	130.4 (3)
C7—N2—C6	106.4 (2)	C11—C16—C15	119.3 (3)
C7—N2—C8	127.9 (2)	C14—C13—C12	121.8 (3)
C6—N2—C8	125.7 (2)	C14—C13—H13	119.1
C2—C3—C4	121.5 (3)	C12—C13—H13	119.1
C2—C3—H3	119.3	C11—C12—C13	116.2 (3)
C4—C3—H3	119.3	C11—C12—H12	121.9
C7—N1—C1	104.1 (2)	C13—C12—H12	121.9
N1—C7—N2	114.3 (3)	C5—C4—C3	121.9 (3)
N1—C7—H7	122.9	C5—C4—H4	119.0
N2—C7—H7	122.9	C3—C4—H4	119.0
C25—N5—C19	106.4 (2)		
N5—C18—C9—C26	69.8 (3)	N5—C19—C24—N6	0.1 (3)
N5—C18—C9—C8	-168.8 (2)	C20—C19—C24—C23	-1.6 (4)
N5—C18—C9—C10	-51.3 (3)	N5—C19—C24—C23	179.8 (2)
C8—C9—C26—Br1	46.0 (3)	N5—C19—C20—C21	178.9 (3)
C18—C9—C26—Br1	164.16 (16)	C24—C19—C20—C21	0.8 (4)
C10—C9—C26—Br1	-77.9 (2)	C22—C21—C20—C19	-0.4 (4)
C26—C9—C10—N3	58.1 (3)	C20—C21—C22—C23	1.0 (5)
C8—C9—C10—N3	-67.7 (3)	C19—N5—C25—N6	-1.9 (3)
C18—C9—C10—N3	175.8 (2)	C18—N5—C25—N6	179.1 (2)
C26—C9—C8—N2	64.9 (3)	N5—C25—N6—C24	1.9 (3)
C18—C9—C8—N2	-53.0 (3)	C19—C24—N6—C25	-1.2 (3)
C10—C9—C8—N2	-169.4 (2)	C23—C24—N6—C25	179.2 (3)
C3—C2—C1—N1	-176.6 (3)	C21—C22—C23—C24	-1.8 (4)
C3—C2—C1—C6	1.8 (4)	N6—C24—C23—C22	-178.3 (3)
C4—C5—C6—N2	177.7 (3)	C19—C24—C23—C22	2.1 (4)
C4—C5—C6—C1	0.7 (4)	C9—C10—N3—C17	-93.6 (3)
N1—C1—C6—N2	-0.9 (3)	C9—C10—N3—C11	90.9 (3)
C2—C1—C6—N2	-179.5 (2)	C17—N3—C11—C12	-174.1 (3)
N1—C1—C6—C5	176.8 (2)	C10—N3—C11—C12	2.1 (4)
C2—C1—C6—C5	-1.8 (4)	C17—N3—C11—C16	2.1 (3)
C5—C6—N2—C7	-176.0 (3)	C10—N3—C11—C16	178.3 (2)
C1—C6—N2—C7	1.4 (3)	C16—C15—C14—C13	-0.3 (5)
C5—C6—N2—C8	1.7 (4)	C16—N4—C17—N3	0.6 (3)
C1—C6—N2—C8	179.1 (2)	C11—N3—C17—N4	-1.7 (3)
C9—C8—N2—C7	-79.6 (3)	C10—N3—C17—N4	-178.1 (2)
C9—C8—N2—C6	103.2 (3)	C17—N4—C16—C11	0.8 (3)
C1—C2—C3—C4	-0.7 (5)	C17—N4—C16—C15	176.5 (3)
C6—C1—N1—C7	0.1 (3)	C12—C11—C16—N4	174.8 (2)
C2—C1—N1—C7	178.5 (3)	N3—C11—C16—N4	-1.8 (3)
C1—N1—C7—N2	0.9 (3)	C12—C11—C16—C15	-1.5 (4)
C6—N2—C7—N1	-1.5 (3)	N3—C11—C16—C15	-178.1 (2)
C8—N2—C7—N1	-179.1 (2)	C14—C15—C16—N4	-174.1 (3)
C9—C18—N5—C25	-77.3 (3)	C14—C15—C16—C11	1.3 (4)



## supporting information

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C9—C18—N5—C19	103.9 (3)	C15—C14—C13—C12	-0.7 (5)
C25—N5—C19—C20	-177.4 (3)	N3—C11—C12—C13	176.1 (3)
C18—N5—C19—C20	1.6 (4)	C16—C11—C12—C13	0.5 (4)
C25—N5—C19—C24	1.0 (3)	C14—C13—C12—C11	0.6 (5)
C18—N5—C19—C24	180.0 (2)	C6—C5—C4—C3	0.4 (4)
C20—C19—C24—N6	178.7 (2)	C2—C3—C4—C5	-0.4 (5)

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