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# 4-(4-Bromophenylhydrazono)-1-(5-bromopyrimidin-2-yl)-3-methyl-2-pyrazolin-5-one

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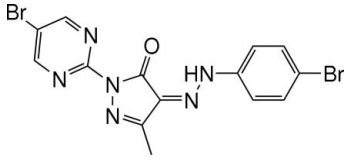
Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.083; $wR$ factor = 0.139; data-to-parameter ratio = 23.0.

The asymmetric unit of the title compound, $C_{14}H_{10}Br_2N_6O$, contains two crystallographically independent molecules. The pyrazole ring of one molecule makes dihedral angles of 22.0 (3) and 3.5 (3)° with the pyrimidine and benzene rings, respectively; the corresponding values in the other molecule are 9.2 (3) and 2.1 (3)°, respectively. The molecules are linked by N—H···O, C—H···N and C—H···Br hydrogen bonds.

## Related literature

For related literature, see: Baraldi *et al.* (1996, 2003); Kalluraya & Rahiman (1997); Kalluraya *et al.* (2001); Lingappa *et al.* (2006, 2007). For related crystal structures, see: Thiruvalluvar, Subramanyam, Kalluraya *et al.* (2007*a*,*b*); Thiruvalluvar, Subramanyam, Lingappa *et al.* (2007).



## Experimental

### Crystal data

$C_{14}H_{10}Br_2N_6O$
$M_r$ = 438.08
Triclinic, $P\overline{1}$
$a$ = 9.1647 (3) Å
$b$ = 12.2833 (5) Å
$c$ = 14.0288 (5) Å
$\alpha$ = 86.532 (3)°
$\beta$ = 84.218 (3)°
$\gamma$ = 78.747 (3)°
$V$ = 1539.67 (10) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 5.28 mm$^{-1}$
$T$ = 200 (2) K
0.44 × 0.39 × 0.28 mm

### Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.205, $T_{max}$ = 0.320 (expected range = 0.146–0.228)
24958 measured reflections
9542 independent reflections
6336 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.139
$S$ = 1.25
9542 reflections
415 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.83 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.64 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N6$A$—H6$A$···O5$A$ | 0.88 | 2.14 | 2.821 (6) | 134 |
| N6$B$—H6$B$···O5$B$ | 0.88 | 2.10 | 2.782 (6) | 134 |
| C13$A$—H13$A$···N12$B^{i}$ | 0.95 | 2.61 | 3.193 (7) | 120 |
| C15$A$—H15$A$···Br4$^{ii}$ | 0.95 | 2.92 | 3.761 (6) | 148 |
| C15$B$—H15$B$···Br2$^{ii}$ | 0.95 | 2.87 | 3.746 (6) | 153 |
| C31$A$—H31$A$···Br3$^{i}$ | 0.98 | 2.88 | 3.858 (6) | 173 |
| C31$B$—H31$D$···Br1$^{i}$ | 0.98 | 2.92 | 3.862 (6) | 160 |
| C45$A$—H45$A$···N16$B^{ii}$ | 0.95 | 2.62 | 3.539 (7) | 162 |

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

RJB acknowledges the NSF-MRI program for funding to purchase the X-ray CCD diffractometer. AT thanks the UGC, India, for the award of a Minor Research Project [file No. MRP-2355/06(UGC-SERO), link No. 2355, 10/01/2007].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2116).

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# supporting information

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## 4-(4-Bromophenylhydrazono)-1-(5-bromopyrimidin-2-yl)-3-methyl-2-pyrazolin-5-one

**M. Subramanyam, B. Lingappa, A. Thiruvalluvar, R. J. Butcher and Balakrishna Kalluraya**

### S1. Comment

The chemistry of pyrimidine and its derivatives has been studied due to their diverse biological activities (Baraldi *et al.*, 1996; Lingappa *et al.*, 2006, 2007). Pyrazoles and their derivatives are found to be associated with diverse pharmacological activities. Pyrazoles constitute an important class of heterocycles, which display interesting biological properties such as fungicidal, anti-inflammatory, anti-arthritic, anti-depressant and antiviral activity (Baraldi *et al.*, 2003; Kalluraya *et al.*, 2001; Kalluraya & Rahiman, 1997). The title compound, has been analysed as part of our crystallographic studies on pyrimidine derivatives (Thiruvalluvar *et al.*, 2007*a*,b; Thiruvalluvar, Subramanyam, Lingappa *et al.*, 2007). The asymmetric unit of the title compound, $C_{14}H_{10}Br_2N_6O$, Fig. 1, contains two crystallographically independent molecules, A and B. The pyrazole ring of A makes dihedral angles of 22.0 (3)° and 3.5 (3)° with the pyrimidine ring and phenyl ring respectively; the corresponding values in molecule B are 9.2 (3)° and 2.1 (3)°. The molecules are linked by N—H···O, C—H···N and C—H···Br hydrogen bonds; see Fig. 2 and hydrogen bond table.

### S2. Experimental

Ethyl-2-(4-bromohydrazono-3-oxobutanoate (3.2 g, 0.01 mol) was dissolved in glacial acetic acid (15 ml). To this a solution of 2-hydrazino-5-bromo-pyrimidine (1.9 g, 0.01 mol) in glacial acetic acid (20 ml) was added and the mixture was refluxed for 4 h in an oil bath. It was cooled and allowed to stand overnight. The separated solid was filtered, dried and then recrystallized from ethanol to give reddish flakes. Further recrystallization from ethyl acetate gave the yellowish red crystals suitable for X-ray analysis (3.0 g, 70%).

### S3. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.88–0.98 Å and $U_{iso}$=1.2 or 1.5 times $U_{eq}$(C).

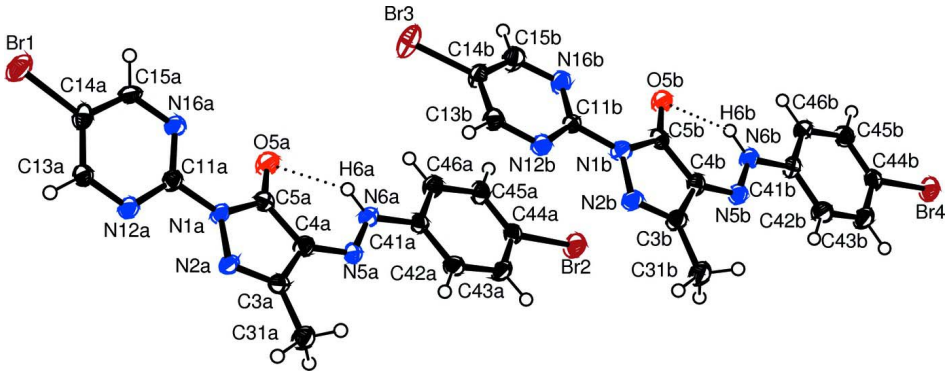


**Figure 1**

The molecular structure of the title compound with the atomic numbering and 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radius.

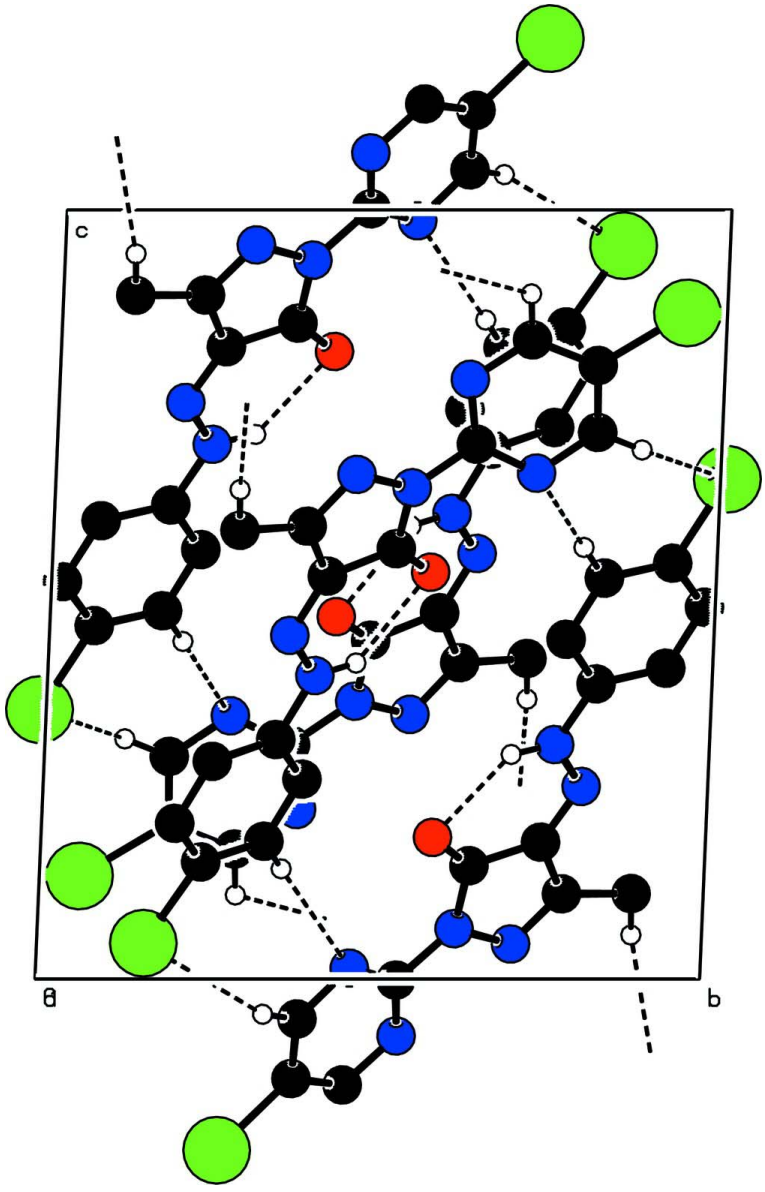


**Figure 2**

The packing of the title compound, viewed down the *a* axis. Dashed lines indicate hydrogen bonds.

**4-(4-Bromophenylhydrazono)-1-(5-bromopyrimidin-2-yl)-3-methyl-2-pyrazolin-5-one**

*Crystal data*

$C_{14}H_{10}Br_2N_6O$
$M_r$ = 438.08
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 9.1647 (3) Å
$b$ = 12.2833 (5) Å
$c$ = 14.0288 (5) Å
$\alpha$ = 86.532 (3)°
$\beta$ = 84.218 (3)°
$\gamma$ = 78.747 (3)°
$V$ = 1539.67 (10) Å$^3$
$Z$ = 4
$F$(000) = 856
$D_x$ = 1.890 Mg m$^{-3}$
Melting point: 534(1) K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5753 reflections
$\theta$ = 4.6–32.4°

$\mu$ = 5.28 mm$^{-1}$
$T$ = 200 K

Prism, pale-yellow
0.44 × 0.39 × 0.28 mm

*Data collection*

Oxford Diffraction Gemini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.5081 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.205, $T_{max}$ = 0.320

24958 measured reflections
9542 independent reflections
6336 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057
$\theta_{max}$ = 32.5°, $\theta_{min}$ = 4.6°
$h$ = −13→13
$k$ = −18→18
$l$ = −20→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.139
$S$ = 1.25
9542 reflections
415 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
$w = 1/[\sigma^2(F_o^2) + (0.0029P)^2 + 9.1374P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.83 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.64 e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.25785 (9) | 0.06030 (5) | 0.13400 (5) | 0.0442 (2) |
| Br2 | 0.35450 (8) | 0.83940 (5) | 0.95346 (4) | 0.0376 (2) |
| O5A | 0.3522 (5) | 0.4304 (3) | 0.4711 (3) | 0.0337 (12) |
| N1A | 0.1660 (5) | 0.4635 (4) | 0.3613 (3) | 0.0230 (12) |
| N2A | 0.0409 (5) | 0.5473 (4) | 0.3440 (3) | 0.0233 (12) |
| N5A | 0.1545 (5) | 0.6383 (4) | 0.5533 (3) | 0.0236 (12) |
| N6A | 0.2645 (5) | 0.5980 (4) | 0.6055 (3) | 0.0272 (14) |
| N12A | 0.1363 (5) | 0.3829 (4) | 0.2204 (3) | 0.0269 (14) |
| N16A | 0.2742 (5) | 0.2773 (4) | 0.3423 (3) | 0.0283 (14) |
| C3A | 0.0276 (6) | 0.6191 (4) | 0.4112 (4) | 0.0241 (16) |
| C4A | 0.1428 (6) | 0.5855 (4) | 0.4762 (4) | 0.0249 (17) |
| C5A | 0.2370 (6) | 0.4835 (4) | 0.4405 (4) | 0.0251 (17) |
| C11A | 0.1945 (6) | 0.3696 (4) | 0.3045 (4) | 0.0233 (17) |
| C13A | 0.1549 (6) | 0.2918 (4) | 0.1690 (4) | 0.0256 (17) |

| | | | | |
|---|---|---|---|---|
| C14A | 0.2345 (6) | 0.1912 (5) | 0.2024 (4) | 0.0267 (17) |
| C15A | 0.2941 (7) | 0.1879 (4) | 0.2893 (4) | 0.0294 (16) |
| C31A | −0.0912 (7) | 0.7199 (5) | 0.4167 (4) | 0.0310 (17) |
| C41A | 0.2811 (6) | 0.6529 (4) | 0.6887 (4) | 0.0218 (14) |
| C42A | 0.1781 (6) | 0.7470 (5) | 0.7170 (4) | 0.0269 (17) |
| C43A | 0.1993 (7) | 0.7997 (5) | 0.7976 (4) | 0.0289 (17) |
| C44A | 0.3238 (6) | 0.7582 (4) | 0.8478 (4) | 0.0240 (16) |
| C45A | 0.4250 (6) | 0.6644 (5) | 0.8210 (4) | 0.0274 (17) |
| C46A | 0.4032 (6) | 0.6110 (5) | 0.7402 (4) | 0.0268 (17) |
| Br3 | 0.35984 (7) | 0.28407 (6) | −0.22267 (5) | 0.0439 (2) |
| Br4 | 0.35687 (7) | 1.01017 (5) | 0.64977 (4) | 0.0352 (2) |
| O5B | 0.3253 (4) | 0.5890 (3) | 0.1841 (3) | 0.0289 (11) |
| N1B | 0.1528 (5) | 0.6272 (4) | 0.0654 (3) | 0.0242 (12) |
| N2B | 0.0319 (5) | 0.7132 (4) | 0.0455 (3) | 0.0257 (12) |
| N5B | 0.1476 (5) | 0.8095 (4) | 0.2504 (3) | 0.0243 (12) |
| N6B | 0.2564 (5) | 0.7670 (4) | 0.3048 (3) | 0.0255 (12) |
| N12B | 0.1135 (5) | 0.5468 (4) | −0.0740 (3) | 0.0246 (12) |
| N16B | 0.3245 (5) | 0.4721 (4) | 0.0142 (3) | 0.0297 (16) |
| C3B | 0.0199 (6) | 0.7867 (5) | 0.1108 (4) | 0.0257 (17) |
| C4B | 0.1306 (6) | 0.7519 (5) | 0.1779 (4) | 0.0243 (16) |
| C5B | 0.2192 (6) | 0.6457 (5) | 0.1473 (4) | 0.0225 (16) |
| C11B | 0.1992 (6) | 0.5427 (4) | −0.0014 (4) | 0.0221 (14) |
| C13B | 0.1610 (6) | 0.4687 (4) | −0.1378 (4) | 0.0253 (17) |
| C14B | 0.2899 (6) | 0.3913 (5) | −0.1295 (4) | 0.0280 (17) |
| C15B | 0.3703 (7) | 0.3965 (5) | −0.0520 (4) | 0.0337 (17) |
| C31B | −0.0924 (7) | 0.8914 (5) | 0.1110 (4) | 0.0378 (19) |
| C41B | 0.2806 (6) | 0.8256 (5) | 0.3837 (4) | 0.0248 (17) |
| C42B | 0.1926 (7) | 0.9294 (5) | 0.4041 (4) | 0.0326 (17) |
| C43B | 0.2166 (7) | 0.9838 (5) | 0.4834 (4) | 0.0327 (17) |
| C44B | 0.3283 (6) | 0.9332 (5) | 0.5407 (4) | 0.0261 (16) |
| C45B | 0.4170 (7) | 0.8313 (5) | 0.5212 (4) | 0.0281 (17) |
| C46B | 0.3920 (6) | 0.7777 (4) | 0.4417 (4) | 0.0258 (16) |
| H6A | 0.32796 | 0.53710 | 0.58914 | 0.0325* |
| H13A | 0.11317 | 0.29614 | 0.10926 | 0.0305* |
| H15A | 0.35103 | 0.11993 | 0.31218 | 0.0351* |
| H31A | −0.15409 | 0.72242 | 0.36379 | 0.0462* |
| H31B | −0.15261 | 0.71796 | 0.47794 | 0.0462* |
| H31C | −0.04557 | 0.78606 | 0.41202 | 0.0462* |
| H42A | 0.09463 | 0.77462 | 0.68162 | 0.0322* |
| H43A | 0.12971 | 0.86348 | 0.81856 | 0.0344* |
| H45A | 0.50800 | 0.63667 | 0.85679 | 0.0324* |
| H46A | 0.47163 | 0.54612 | 0.72037 | 0.0320* |
| H6B | 0.31353 | 0.70229 | 0.29195 | 0.0304* |
| H13B | 0.10427 | 0.46644 | −0.19044 | 0.0301* |
| H15B | 0.46075 | 0.34463 | −0.04581 | 0.0402* |
| H31D | −0.15362 | 0.89370 | 0.05723 | 0.0567* |
| H31E | −0.15657 | 0.89487 | 0.17142 | 0.0567* |
| H31F | −0.04134 | 0.95486 | 0.10445 | 0.0567* |

| | | | | |
|---|---|---|---|---|
| H42B | 0.11701 | 0.96245 | 0.36400 | 0.0391* |
| H43B | 0.15775 | 1.05438 | 0.49828 | 0.0397* |
| H45B | 0.49313 | 0.79874 | 0.56111 | 0.0337* |
| H46B | 0.45184 | 0.70742 | 0.42684 | 0.0303* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0592 (4) | 0.0278 (3) | 0.0472 (4) | −0.0018 (3) | −0.0158 (3) | −0.0168 (3) |
| Br2 | 0.0477 (4) | 0.0328 (3) | 0.0341 (3) | −0.0035 (3) | −0.0141 (3) | −0.0127 (3) |
| O5A | 0.036 (2) | 0.031 (2) | 0.034 (2) | 0.0029 (19) | −0.0159 (19) | −0.0093 (18) |
| N1A | 0.026 (2) | 0.020 (2) | 0.023 (2) | 0.0008 (19) | −0.0097 (18) | −0.0067 (18) |
| N2A | 0.026 (2) | 0.018 (2) | 0.025 (2) | −0.0002 (19) | −0.0041 (18) | −0.0041 (18) |
| N5A | 0.028 (2) | 0.023 (2) | 0.020 (2) | −0.003 (2) | −0.0056 (18) | −0.0030 (18) |
| N6A | 0.033 (3) | 0.022 (2) | 0.025 (2) | 0.001 (2) | −0.005 (2) | −0.0042 (19) |
| N12A | 0.032 (3) | 0.023 (2) | 0.026 (2) | −0.001 (2) | −0.010 (2) | −0.0059 (19) |
| N16A | 0.035 (3) | 0.023 (2) | 0.025 (2) | 0.004 (2) | −0.011 (2) | −0.0035 (19) |
| C3A | 0.028 (3) | 0.020 (2) | 0.024 (3) | −0.003 (2) | −0.005 (2) | 0.001 (2) |
| C4A | 0.029 (3) | 0.021 (3) | 0.026 (3) | −0.007 (2) | −0.002 (2) | −0.004 (2) |
| C5A | 0.031 (3) | 0.022 (3) | 0.022 (3) | −0.003 (2) | −0.005 (2) | 0.000 (2) |
| C11A | 0.025 (3) | 0.022 (3) | 0.024 (3) | −0.005 (2) | −0.004 (2) | −0.005 (2) |
| C13A | 0.029 (3) | 0.025 (3) | 0.023 (3) | −0.002 (2) | −0.008 (2) | −0.004 (2) |
| C14A | 0.029 (3) | 0.029 (3) | 0.026 (3) | −0.012 (2) | −0.004 (2) | −0.008 (2) |
| C15A | 0.037 (3) | 0.016 (2) | 0.034 (3) | 0.002 (2) | −0.012 (3) | 0.000 (2) |
| C31A | 0.032 (3) | 0.029 (3) | 0.032 (3) | −0.002 (3) | −0.007 (2) | −0.007 (2) |
| C41A | 0.026 (3) | 0.021 (2) | 0.019 (2) | −0.005 (2) | −0.003 (2) | −0.002 (2) |
| C42A | 0.029 (3) | 0.025 (3) | 0.026 (3) | −0.001 (2) | −0.008 (2) | −0.001 (2) |
| C43A | 0.034 (3) | 0.021 (3) | 0.030 (3) | 0.002 (2) | −0.005 (2) | −0.008 (2) |
| C44A | 0.031 (3) | 0.023 (3) | 0.019 (2) | −0.006 (2) | −0.004 (2) | −0.003 (2) |
| C45A | 0.026 (3) | 0.033 (3) | 0.024 (3) | −0.005 (2) | −0.005 (2) | −0.005 (2) |
| C46A | 0.025 (3) | 0.029 (3) | 0.027 (3) | −0.004 (2) | −0.004 (2) | −0.006 (2) |
| Br3 | 0.0343 (3) | 0.0493 (4) | 0.0480 (4) | 0.0003 (3) | −0.0035 (3) | −0.0294 (3) |
| Br4 | 0.0448 (4) | 0.0345 (3) | 0.0278 (3) | −0.0061 (3) | −0.0067 (3) | −0.0123 (2) |
| O5B | 0.033 (2) | 0.029 (2) | 0.0251 (19) | −0.0004 (18) | −0.0116 (17) | −0.0067 (16) |
| N1B | 0.023 (2) | 0.023 (2) | 0.027 (2) | −0.0024 (19) | −0.0071 (18) | −0.0026 (19) |
| N2B | 0.024 (2) | 0.024 (2) | 0.027 (2) | 0.003 (2) | −0.0061 (19) | −0.0031 (19) |
| N5B | 0.026 (2) | 0.024 (2) | 0.023 (2) | −0.003 (2) | −0.0044 (18) | −0.0050 (18) |
| N6B | 0.028 (2) | 0.025 (2) | 0.023 (2) | −0.001 (2) | −0.0056 (19) | −0.0060 (18) |
| N12B | 0.026 (2) | 0.023 (2) | 0.025 (2) | −0.003 (2) | −0.0058 (18) | −0.0033 (18) |
| N16B | 0.030 (3) | 0.034 (3) | 0.023 (2) | 0.003 (2) | −0.0068 (19) | −0.006 (2) |
| C3B | 0.023 (3) | 0.026 (3) | 0.027 (3) | 0.000 (2) | −0.005 (2) | −0.004 (2) |
| C4B | 0.027 (3) | 0.027 (3) | 0.020 (2) | −0.006 (2) | −0.003 (2) | −0.006 (2) |
| C5B | 0.024 (3) | 0.027 (3) | 0.018 (2) | −0.007 (2) | −0.005 (2) | −0.001 (2) |
| C11B | 0.024 (3) | 0.021 (2) | 0.020 (2) | 0.000 (2) | −0.003 (2) | −0.002 (2) |
| C13B | 0.028 (3) | 0.024 (3) | 0.025 (3) | −0.005 (2) | −0.006 (2) | −0.004 (2) |
| C14B | 0.025 (3) | 0.029 (3) | 0.028 (3) | 0.001 (2) | 0.001 (2) | −0.010 (2) |
| C15B | 0.026 (3) | 0.038 (3) | 0.033 (3) | 0.009 (3) | −0.009 (2) | −0.007 (3) |
| C31B | 0.041 (4) | 0.039 (3) | 0.029 (3) | 0.009 (3) | −0.009 (3) | −0.011 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C41B | 0.025 (3) | 0.027 (3) | 0.022 (3) | −0.003 (2) | 0.000 (2) | −0.007 (2) |
| C42B | 0.038 (3) | 0.031 (3) | 0.028 (3) | 0.000 (3) | −0.011 (3) | −0.003 (2) |
| C43B | 0.037 (3) | 0.028 (3) | 0.031 (3) | 0.002 (3) | −0.004 (3) | −0.009 (2) |
| C44B | 0.032 (3) | 0.029 (3) | 0.018 (2) | −0.008 (3) | −0.001 (2) | −0.002 (2) |
| C45B | 0.029 (3) | 0.032 (3) | 0.023 (3) | −0.003 (3) | −0.006 (2) | −0.002 (2) |
| C46B | 0.031 (3) | 0.021 (2) | 0.025 (3) | −0.004 (2) | −0.002 (2) | −0.003 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C14A | 1.888 (6) | C41A—C46A | 1.390 (8) |
| Br2—C44A | 1.909 (5) | C41A—C42A | 1.392 (8) |
| Br3—C14B | 1.888 (6) | C42A—C43A | 1.385 (8) |
| Br4—C44B | 1.912 (6) | C43A—C44A | 1.396 (8) |
| O5A—C5A | 1.230 (7) | C44A—C45A | 1.376 (8) |
| O5B—C5B | 1.221 (7) | C45A—C46A | 1.394 (8) |
| N1A—N2A | 1.414 (7) | C13A—H13A | 0.9500 |
| N1A—C11A | 1.409 (7) | C15A—H15A | 0.9500 |
| N1A—C5A | 1.400 (7) | C31A—H31A | 0.9800 |
| N2A—C3A | 1.310 (7) | C31A—H31C | 0.9800 |
| N5A—N6A | 1.307 (6) | C31A—H31B | 0.9800 |
| N5A—C4A | 1.318 (7) | C42A—H42A | 0.9500 |
| N6A—C41A | 1.418 (7) | C43A—H43A | 0.9500 |
| N12A—C11A | 1.331 (7) | C45A—H45A | 0.9500 |
| N12A—C13A | 1.342 (7) | C46A—H46A | 0.9500 |
| N16A—C11A | 1.335 (7) | C3B—C4B | 1.440 (8) |
| N16A—C15A | 1.336 (7) | C3B—C31B | 1.482 (9) |
| N6A—H6A | 0.8800 | C4B—C5B | 1.459 (8) |
| N1B—N2B | 1.411 (7) | C13B—C14B | 1.374 (8) |
| N1B—C11B | 1.415 (7) | C14B—C15B | 1.385 (8) |
| N1B—C5B | 1.403 (7) | C41B—C46B | 1.388 (8) |
| N2B—C3B | 1.307 (7) | C41B—C42B | 1.398 (9) |
| N5B—C4B | 1.312 (7) | C42B—C43B | 1.389 (8) |
| N5B—N6B | 1.323 (6) | C43B—C44B | 1.392 (8) |
| N6B—C41B | 1.414 (7) | C44B—C45B | 1.379 (9) |
| N12B—C13B | 1.332 (7) | C45B—C46B | 1.389 (8) |
| N12B—C11B | 1.340 (7) | C13B—H13B | 0.9500 |
| N16B—C15B | 1.332 (7) | C15B—H15B | 0.9500 |
| N16B—C11B | 1.326 (7) | C31B—H31D | 0.9800 |
| N6B—H6B | 0.8800 | C31B—H31E | 0.9800 |
| C3A—C31A | 1.481 (8) | C31B—H31F | 0.9800 |
| C3A—C4A | 1.447 (8) | C42B—H42B | 0.9500 |
| C4A—C5A | 1.460 (7) | C43B—H43B | 0.9500 |
| C13A—C14A | 1.388 (8) | C45B—H45B | 0.9500 |
| C14A—C15A | 1.381 (8) | C46B—H46B | 0.9500 |
| | | | |
| Br1···Br2$^{i}$ | 3.7421 (9) | C5B···N2A | 3.347 (7) |
| Br2···C15B$^{ii}$ | 3.746 (6) | C11B···C45A$^{x}$ | 3.527 (8) |
| Br2···Br1$^{iii}$ | 3.7421 (9) | C11B···C44A$^{x}$ | 3.578 (7) |

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|---|---|---|---|
| Br2···C3B$^{iv}$ | 3.733 (6) | C11B···N12B$^{v}$ | 3.319 (7) |
| Br3···C31B$^{v}$ | 3.740 (6) | C13A···C42A$^{ix}$ | 3.405 (8) |
| Br3···N6B$^{vi}$ | 3.536 (5) | C13A···N12B$^{v}$ | 3.193 (7) |
| Br3···C46B$^{vi}$ | 3.659 (6) | C13B···C41A$^{x}$ | 3.467 (8) |
| Br4···C45B$^{vii}$ | 3.721 (6) | C13B···N2B$^{v}$ | 3.244 (7) |
| Br4···C43A | 3.644 (6) | C13B···N1B$^{v}$ | 3.358 (7) |
| Br1···H31D$^{v}$ | 2.9200 | C13B···C46A$^{x}$ | 3.361 (8) |
| Br2···H15B$^{ii}$ | 2.8700 | C13B···N12A$^{v}$ | 3.245 (7) |
| Br3···H6B$^{vi}$ | 3.0900 | C14B···C46A$^{x}$ | 3.438 (8) |
| Br3···H46B$^{vi}$ | 3.2000 | C15B···O5B$^{vi}$ | 3.219 (7) |
| Br3···H31E$^{v}$ | 3.1600 | C15B···Br2$^{ii}$ | 3.746 (6) |
| Br3···H31A$^{v}$ | 2.8800 | C31A···C5A$^{ix}$ | 3.493 (8) |
| Br4···H31E$^{viii}$ | 3.1000 | C31A···N5B | 3.323 (8) |
| Br4···H15A$^{ii}$ | 2.9200 | C31B···Br3$^{v}$ | 3.740 (6) |
| O5A···N5A | 3.044 (6) | C41A···C45B | 3.425 (8) |
| O5A···C46B$^{ii}$ | 3.375 (7) | C41A···C13B$^{iv}$ | 3.467 (8) |
| O5A···N6A | 2.821 (6) | C41B···C4A | 3.555 (8) |
| O5A···N16A | 2.917 (6) | C42A···C13A$^{ix}$ | 3.405 (8) |
| O5B···N16B | 2.857 (6) | C42A···C45B | 3.569 (8) |
| O5B···N5B | 3.022 (6) | C43A···Br4 | 3.644 (6) |
| O5B···N6B | 2.782 (6) | C44A···C11B$^{iv}$ | 3.578 (7) |
| O5B···C15B$^{vi}$ | 3.219 (7) | C45A···C11B$^{iv}$ | 3.527 (8) |
| O5B···N1A | 3.220 (6) | C45B···Br4$^{vii}$ | 3.721 (6) |
| O5B···C46A$^{ii}$ | 3.344 (7) | C45B···C41A | 3.425 (8) |
| O5A···H46B$^{ii}$ | 2.6800 | C45B···C42A | 3.569 (8) |
| O5A···H6A | 2.1400 | C46A···C13B$^{iv}$ | 3.361 (8) |
| O5A···H31B$^{ix}$ | 2.8400 | C46A···C14B$^{iv}$ | 3.438 (8) |
| O5B···H6B | 2.1000 | C46A···O5B$^{ii}$ | 3.344 (7) |
| O5B···H46A$^{ii}$ | 2.6500 | C46B···N5A | 3.250 (7) |
| O5B···H15B$^{vi}$ | 2.8200 | C46B···O5A$^{ii}$ | 3.375 (7) |
| N1A···O5B | 3.220 (6) | C46B···N6A | 3.372 (7) |
| N1B···C13B$^{v}$ | 3.358 (7) | C46B···C4A | 3.573 (7) |
| N2A···N12A | 2.698 (6) | C46B···Br3$^{vi}$ | 3.659 (6) |
| N2A···C5B | 3.347 (7) | C5A···H6A | 2.4900 |
| N2A···C4A$^{ix}$ | 3.402 (7) | C5A···H31B$^{ix}$ | 2.8700 |
| N2B···N12B | 2.667 (6) | C5B···H6B | 2.4700 |
| N2B···C13B$^{v}$ | 3.244 (7) | C15A···H45B$^{ii}$ | 3.0400 |
| N5A···C46B | 3.250 (7) | C15B···H45A$^{ii}$ | 3.0400 |
| N5A···O5A | 3.044 (6) | C31A···H43B$^{viii}$ | 3.0100 |
| N5B···O5B | 3.022 (6) | C42B···H31C | 3.0500 |
| N5B···C31A | 3.323 (8) | H6A···C5A | 2.4900 |
| N5B···C3A | 3.411 (7) | H6A···H46A | 2.3900 |
| N6A···C46B | 3.372 (7) | H6A···O5A | 2.1400 |
| N6A···O5A | 2.821 (6) | H6B···H46B | 2.3900 |
| N6B···C4A | 3.404 (7) | H6B···O5B | 2.1000 |
| N6B···Br3$^{vi}$ | 3.536 (5) | H6B···C5B | 2.4700 |
| N6B···C3A | 3.233 (7) | H6B···Br3$^{vi}$ | 3.0900 |
| N6B···O5B | 2.782 (6) | H13A···N2B$^{v}$ | 2.6800 |

| | | | |
|---|---|---|---|
| N12A···C13B$^{v}$ | 3.245 (7) | H13A···N12B$^{v}$ | 2.6100 |
| N12A···N12B$^{v}$ | 3.188 (6) | H13B···N12A$^{v}$ | 2.6400 |
| N12A···N2A | 2.698 (6) | H13B···N2A$^{v}$ | 2.6700 |
| N12B···N2B | 2.667 (6) | H15A···Br4$^{ii}$ | 2.9200 |
| N12B···C13A$^{v}$ | 3.193 (7) | H15B···O5B$^{vi}$ | 2.8200 |
| N12B···C11B$^{v}$ | 3.319 (7) | H15B···Br2$^{ii}$ | 2.8700 |
| N12B···N12A$^{v}$ | 3.188 (6) | H31A···Br3$^{v}$ | 2.8800 |
| N12B···N12B$^{v}$ | 3.120 (6) | H31B···N16A$^{ix}$ | 2.6500 |
| N16A···O5A | 2.917 (6) | H31B···C5A$^{ix}$ | 2.8700 |
| N16B···O5B | 2.857 (6) | H31B···O5A$^{ix}$ | 2.8400 |
| N2A···H13B$^{v}$ | 2.6700 | H31C···N5B | 2.7700 |
| N2B···H13A$^{v}$ | 2.6800 | H31C···C42B | 3.0500 |
| N5A···H42A | 2.4800 | H31C···H43B$^{viii}$ | 2.3900 |
| N5B···H42B | 2.4900 | H31D···Br1$^{v}$ | 2.9200 |
| N5B···H31C | 2.7700 | H31E···Br4$^{viii}$ | 3.1000 |
| N12A···H13B$^{v}$ | 2.6400 | H31E···Br3$^{v}$ | 3.1600 |
| N12B···H13A$^{v}$ | 2.6100 | H31F···H43A$^{viii}$ | 2.4900 |
| N16A···H45B$^{ii}$ | 2.6300 | H42A···N5A | 2.4800 |
| N16A···H31B$^{ix}$ | 2.6500 | H42B···N5B | 2.4900 |
| N16B···H45A$^{ii}$ | 2.6200 | H43A···H31F$^{viii}$ | 2.4900 |
| C3A···N5B | 3.411 (7) | H43B···H31C$^{viii}$ | 2.3900 |
| C3A···C4A$^{ix}$ | 3.436 (7) | H43B···C31A$^{viii}$ | 3.0100 |
| C3A···C5A$^{ix}$ | 3.414 (8) | H45A···C15B$^{ii}$ | 3.0400 |
| C3A···N6B | 3.233 (7) | H45A···N16B$^{ii}$ | 2.6200 |
| C3B···Br2$^{x}$ | 3.733 (6) | H45B···C15A$^{ii}$ | 3.0400 |
| C4A···N6B | 3.404 (7) | H45B···N16A$^{ii}$ | 2.6300 |
| C4A···N2A$^{ix}$ | 3.402 (7) | H46A···O5B$^{ii}$ | 2.6500 |
| C4A···C41B | 3.555 (8) | H46A···H6A | 2.3900 |
| C4A···C46B | 3.573 (7) | H46B···H6B | 2.3900 |
| C4A···C3A$^{ix}$ | 3.436 (7) | H46B···Br3$^{vi}$ | 3.2000 |
| C5A···C31A$^{ix}$ | 3.493 (8) | H46B···O5A$^{ii}$ | 2.6800 |
| C5A···C3A$^{ix}$ | 3.414 (8) | | |

| | | | |
|---|---|---|---|
| N2A—N1A—C5A | 112.8 (4) | H31B—C31A—H31C | 109.00 |
| N2A—N1A—C11A | 117.8 (4) | H31A—C31A—H31C | 109.00 |
| C5A—N1A—C11A | 129.2 (5) | C43A—C42A—H42A | 120.00 |
| N1A—N2A—C3A | 106.9 (4) | C41A—C42A—H42A | 121.00 |
| N6A—N5A—C4A | 118.1 (5) | C42A—C43A—H43A | 120.00 |
| N5A—N6A—C41A | 119.7 (5) | C44A—C43A—H43A | 120.00 |
| C11A—N12A—C13A | 116.3 (5) | C44A—C45A—H45A | 121.00 |
| C11A—N16A—C15A | 115.1 (5) | C46A—C45A—H45A | 121.00 |
| C41A—N6A—H6A | 120.00 | C41A—C46A—H46A | 120.00 |
| N5A—N6A—H6A | 120.00 | C45A—C46A—H46A | 120.00 |
| N2B—N1B—C5B | 112.4 (4) | N2B—C3B—C31B | 122.6 (5) |
| C5B—N1B—C11B | 129.1 (5) | N2B—C3B—C4B | 110.7 (5) |
| N2B—N1B—C11B | 118.2 (4) | C4B—C3B—C31B | 126.7 (5) |
| N1B—N2B—C3B | 107.2 (4) | N5B—C4B—C5B | 128.2 (5) |
| N6B—N5B—C4B | 117.4 (5) | N5B—C4B—C3B | 124.6 (5) |

| | | | |
|---|---|---|---|
| N5B—N6B—C41B | 119.9 (5) | C3B—C4B—C5B | 107.2 (5) |
| C11B—N12B—C13B | 115.0 (5) | O5B—C5B—C4B | 128.0 (5) |
| C11B—N16B—C15B | 114.9 (5) | N1B—C5B—C4B | 102.5 (5) |
| C41B—N6B—H6B | 120.00 | O5B—C5B—N1B | 129.5 (5) |
| N5B—N6B—H6B | 120.00 | N12B—C11B—N16B | 128.5 (5) |
| N2A—C3A—C31A | 122.8 (5) | N1B—C11B—N12B | 115.7 (5) |
| C4A—C3A—C31A | 126.4 (5) | N1B—C11B—N16B | 115.8 (5) |
| N2A—C3A—C4A | 110.8 (5) | N12B—C13B—C14B | 121.8 (5) |
| C3A—C4A—C5A | 106.9 (5) | C13B—C14B—C15B | 117.9 (5) |
| N5A—C4A—C5A | 128.3 (5) | Br3—C14B—C15B | 120.7 (4) |
| N5A—C4A—C3A | 124.9 (5) | Br3—C14B—C13B | 121.4 (4) |
| O5A—C5A—C4A | 128.5 (5) | N16B—C15B—C14B | 121.9 (6) |
| N1A—C5A—C4A | 102.7 (4) | C42B—C41B—C46B | 120.3 (5) |
| O5A—C5A—N1A | 128.9 (5) | N6B—C41B—C42B | 120.8 (5) |
| N1A—C11A—N16A | 116.1 (5) | N6B—C41B—C46B | 118.9 (5) |
| N12A—C11A—N16A | 127.8 (5) | C41B—C42B—C43B | 119.5 (6) |
| N1A—C11A—N12A | 116.2 (5) | C42B—C43B—C44B | 118.9 (6) |
| N12A—C13A—C14A | 120.5 (5) | Br4—C44B—C45B | 120.0 (4) |
| Br1—C14A—C15A | 120.0 (4) | Br4—C44B—C43B | 117.7 (4) |
| C13A—C14A—C15A | 118.2 (5) | C43B—C44B—C45B | 122.4 (5) |
| Br1—C14A—C13A | 121.8 (4) | C44B—C45B—C46B | 118.2 (5) |
| N16A—C15A—C14A | 122.0 (5) | C41B—C46B—C45B | 120.7 (5) |
| C42A—C41A—C46A | 121.2 (5) | N12B—C13B—H13B | 119.00 |
| N6A—C41A—C46A | 118.3 (5) | C14B—C13B—H13B | 119.00 |
| N6A—C41A—C42A | 120.5 (5) | N16B—C15B—H15B | 119.00 |
| C41A—C42A—C43A | 119.0 (5) | C14B—C15B—H15B | 119.00 |
| C42A—C43A—C44A | 119.4 (5) | C3B—C31B—H31D | 109.00 |
| Br2—C44A—C43A | 117.7 (4) | C3B—C31B—H31E | 109.00 |
| Br2—C44A—C45A | 120.3 (4) | C3B—C31B—H31F | 109.00 |
| C43A—C44A—C45A | 122.0 (5) | H31D—C31B—H31E | 109.00 |
| C44A—C45A—C46A | 118.6 (5) | H31D—C31B—H31F | 109.00 |
| C41A—C46A—C45A | 119.8 (5) | H31E—C31B—H31F | 109.00 |
| N12A—C13A—H13A | 120.00 | C41B—C42B—H42B | 120.00 |
| C14A—C13A—H13A | 120.00 | C43B—C42B—H42B | 120.00 |
| N16A—C15A—H15A | 119.00 | C42B—C43B—H43B | 121.00 |
| C14A—C15A—H15A | 119.00 | C44B—C43B—H43B | 121.00 |
| C3A—C31A—H31A | 109.00 | C44B—C45B—H45B | 121.00 |
| H31A—C31A—H31B | 109.00 | C46B—C45B—H45B | 121.00 |
| C3A—C31A—H31B | 109.00 | C41B—C46B—H46B | 120.00 |
| C3A—C31A—H31C | 109.00 | C45B—C46B—H46B | 120.00 |

| | | | |
|---|---|---|---|
| C5A—N1A—N2A—C3A | −1.5 (6) | C15B—N16B—C11B—N1B | −176.9 (5) |
| C11A—N1A—N2A—C3A | 173.3 (5) | N2A—C3A—C4A—N5A | −176.9 (5) |
| N2A—N1A—C5A—O5A | −175.7 (5) | N2A—C3A—C4A—C5A | 1.9 (6) |
| N2A—N1A—C5A—C4A | 2.5 (6) | C31A—C3A—C4A—N5A | 3.2 (9) |
| C11A—N1A—C5A—O5A | 10.3 (9) | C31A—C3A—C4A—C5A | −178.0 (5) |
| C11A—N1A—C5A—C4A | −171.5 (5) | N5A—C4A—C5A—O5A | −5.6 (10) |
| N2A—N1A—C11A—N12A | 22.2 (7) | N5A—C4A—C5A—N1A | 176.2 (5) |

| | | | |
|---|---|---|---|
| N2A—N1A—C11A—N16A | −156.5 (5) | C3A—C4A—C5A—O5A | 175.7 (6) |
| C5A—N1A—C11A—N12A | −164.1 (5) | C3A—C4A—C5A—N1A | −2.6 (6) |
| C5A—N1A—C11A—N16A | 17.2 (8) | N12A—C13A—C14A—Br1 | 178.0 (4) |
| N1A—N2A—C3A—C4A | −0.4 (6) | N12A—C13A—C14A—C15A | −0.3 (8) |
| N1A—N2A—C3A—C31A | 179.6 (5) | C13A—C14A—C15A—N16A | 1.6 (9) |
| C4A—N5A—N6A—C41A | 179.7 (5) | Br1—C14A—C15A—N16A | −176.7 (4) |
| N6A—N5A—C4A—C3A | 179.9 (5) | N6A—C41A—C46A—C45A | 178.5 (5) |
| N6A—N5A—C4A—C5A | 1.3 (8) | N6A—C41A—C42A—C43A | −178.8 (5) |
| N5A—N6A—C41A—C42A | 2.3 (8) | C42A—C41A—C46A—C45A | −0.9 (9) |
| N5A—N6A—C41A—C46A | −177.0 (5) | C46A—C41A—C42A—C43A | 0.5 (9) |
| C13A—N12A—C11A—N1A | −175.8 (5) | C41A—C42A—C43A—C44A | 0.7 (9) |
| C13A—N12A—C11A—N16A | 2.8 (8) | C42A—C43A—C44A—Br2 | 176.1 (4) |
| C11A—N12A—C13A—C14A | −1.7 (8) | C42A—C43A—C44A—C45A | −1.6 (9) |
| C15A—N16A—C11A—N1A | 177.0 (5) | C43A—C44A—C45A—C46A | 1.2 (9) |
| C15A—N16A—C11A—N12A | −1.5 (9) | Br2—C44A—C45A—C46A | −176.4 (4) |
| C11A—N16A—C15A—C14A | −0.8 (8) | C44A—C45A—C46A—C41A | 0.0 (8) |
| C5B—N1B—C11B—N16B | −1.4 (8) | N2B—C3B—C4B—N5B | 178.8 (5) |
| C11B—N1B—N2B—C3B | −173.3 (5) | N2B—C3B—C4B—C5B | 0.8 (7) |
| N2B—N1B—C5B—O5B | −179.6 (6) | C31B—C3B—C4B—N5B | 0.1 (9) |
| N2B—N1B—C5B—C4B | −0.4 (6) | C31B—C3B—C4B—C5B | −178.0 (5) |
| C11B—N1B—C5B—O5B | −6.2 (10) | N5B—C4B—C5B—O5B | 1.1 (10) |
| C11B—N1B—C5B—C4B | 173.0 (5) | N5B—C4B—C5B—N1B | −178.2 (6) |
| N2B—N1B—C11B—N12B | −6.1 (7) | C3B—C4B—C5B—O5B | 179.1 (6) |
| C5B—N1B—N2B—C3B | 0.9 (6) | C3B—C4B—C5B—N1B | −0.2 (6) |
| C5B—N1B—C11B—N12B | −179.2 (5) | N12B—C13B—C14B—Br3 | −177.8 (4) |
| N2B—N1B—C11B—N16B | 171.7 (5) | N12B—C13B—C14B—C15B | 0.1 (8) |
| N1B—N2B—C3B—C31B | 177.8 (5) | Br3—C14B—C15B—N16B | 179.2 (4) |
| N1B—N2B—C3B—C4B | −1.0 (6) | C13B—C14B—C15B—N16B | 1.3 (9) |
| C4B—N5B—N6B—C41B | 179.7 (5) | N6B—C41B—C42B—C43B | 178.5 (5) |
| N6B—N5B—C4B—C3B | −178.9 (5) | C46B—C41B—C42B—C43B | −0.6 (9) |
| N6B—N5B—C4B—C5B | −1.3 (9) | N6B—C41B—C46B—C45B | −178.5 (5) |
| N5B—N6B—C41B—C42B | −1.3 (8) | C42B—C41B—C46B—C45B | 0.6 (9) |
| N5B—N6B—C41B—C46B | 177.8 (5) | C41B—C42B—C43B—C44B | 0.0 (9) |
| C13B—N12B—C11B—N16B | 0.7 (8) | C42B—C43B—C44B—Br4 | −179.5 (5) |
| C11B—N12B—C13B—C14B | −1.0 (8) | C42B—C43B—C44B—C45B | 0.5 (9) |
| C13B—N12B—C11B—N1B | 178.1 (5) | Br4—C44B—C45B—C46B | 179.5 (4) |
| C15B—N16B—C11B—N12B | 0.6 (8) | C43B—C44B—C45B—C46B | −0.5 (9) |
| C11B—N16B—C15B—C14B | −1.6 (8) | C44B—C45B—C46B—C41B | −0.1 (9) |

Symmetry codes: (i) *x*, *y*−1, *z*−1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*+1, *z*+1; (iv) *x*, *y*, *z*+1; (v) −*x*, −*y*+1, −*z*; (vi) −*x*+1, −*y*+1, −*z*; (vii) −*x*+1, −*y*+2, −*z*+1; (viii) −*x*, −*y*+2, −*z*+1; (ix) −*x*, −*y*+1, −*z*+1; (x) *x*, *y*, *z*−1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N6*A*—H6*A*···O5*A* | 0.88 | 2.14 | 2.821 (6) | 134 |
| N6*B*—H6*B*···O5*B* | 0.88 | 2.10 | 2.782 (6) | 134 |
| C13*A*—H13*A*···N12*B*$^{v}$ | 0.95 | 2.61 | 3.193 (7) | 120 |
| C15*A*—H15*A*···Br4$^{ii}$ | 0.95 | 2.92 | 3.761 (6) | 148 |

| | | | | |
|---|---|---|---|---|
| C15*B*—H15*B*···Br2$^{ii}$ | 0.95 | 2.87 | 3.746 (6) | 153 |
| C31*A*—H31*A*···Br3$^{v}$ | 0.98 | 2.88 | 3.858 (6) | 173 |
| C31*B*—H31*D*···Br1$^{v}$ | 0.98 | 2.92 | 3.862 (6) | 160 |
| C45*A*—H45*A*···N16*B*$^{ii}$ | 0.95 | 2.62 | 3.539 (7) | 162 |

Symmetry codes: (ii) $-x+1, -y+1, -z+1$; (v) $-x, -y+1, -z$.