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# 3-[(2*E*)-2-(Butan-2-ylidene)hydrazinyl]-6-chloropyridazine

**Abdul Qayyum Ather,[a,b] M. Nawaz Tahir,[c]* Misbahul Ain Khan[a] and Muhammad Makshoof Athar[d]**

[a]Department of Chemistry, Islamia University, Bahawalpur, Pakistan, [b]Applied Chemistry Research Center, PCSIR Laboratories Complex, Lahore 54600, Pakistan, [c]University of Sargodha, Department of Physics, Sargodha, Pakistan, and [d]Institute of Chemistry, University of the Punjab, Lahore, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

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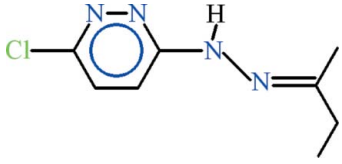
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.035; $wR$ factor = 0.099; data-to-parameter ratio = 15.0.

The asymmetric unit of the title compound, $C_8H_{11}ClN_4$, contains two independent molecules (*A* and *B*) with slightly different conformations: the dihedral angles between the 3-chloro-6-hydrazinylpyridazine units and butyl side chains are 4.5 (2) and 11.98 (16)°. In the crystal, the *A* and *B* molecules are linked by a pair of N—H···N hydrogen bonds, generating an $R_2^2(8)$ loop.

## Related literature

For related structures, see: Ather *et al.* (2009, 2010). For graph-set notation, see: Bernstein *et al.* (1995).



## Experimental

### *Crystal data*

$C_8H_{11}ClN_4$
$M_r$ = 198.66
Triclinic, $P\overline{1}$
$a$ = 8.0623 (4) Å
$b$ = 11.6768 (5) Å
$c$ = 12.1314 (5) Å
$\alpha$ = 113.858 (1)°
$\beta$ = 91.370 (2)°
$\gamma$ = 104.880 (2)°
$V$ = 998.85 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.34 mm$^{-1}$
$T$ = 296 K
0.25 × 0.15 × 0.14 mm

### *Data collection*

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.982, $T_{max}$ = 0.988
14983 measured reflections
3585 independent reflections
2652 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
$S$ = 1.05
3585 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3*A*···N6$^{i}$ | 0.86 | 2.30 | 3.0674 (15) | 148 |
| N7—H7···N2$^{i}$ | 0.86 | 2.24 | 3.0689 (15) | 161 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. They also acknowledge the technical support provided by Bana International, Karachi, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5623).

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# supporting information

*Acta Cryst.* (2010). E**66**, o2499 [doi:10.1107/S160053681003504X]

## 3-[(2*E*)-2-(Butan-2-ylidene)hydrazinyl]-6-chloropyridazine

**Abdul Qayyum Ather, M. Nawaz Tahir, Misbahul Ain Khan and Muhammad Makshoof Athar**

### S1. Comment

In continuation of our studies of pyrazolylpyridazine derivatives (Ather *et al.*, 2009, 2010), the title compound (I, Fig. 1) is being reported here.

The title compound (I), consists of two independent molecules. In one molecule, the 3-chloro-6-hydrazinylpyridazine moiety A (C1—C4/N1—N4/CL1) and the butane group B (C5—C8) is planar with r. m. s. deviation of 0.0217 and 0.0130 Å. The dihedral angle between A/B is 4.53 (24)°. In second molecule, the 3-chloro-6-hydrazinylpyridazine moiety C (C9—C12/N5—N8/CL2) and the butane group D (C13—C16) is planar with r. m. s. deviation of 0.0453 and 0.0446 Å. The dihedral angle between C/D is 11.98 (16)°. The title compound consists of dimers due to N—H···N type of H-bonding (Table 1, Fig. 2) with $R_2^2(8)$ ring motif (Bernstein *et al.*, 1995).

### S2. Experimental

3-Chloro-6-hydrazinylpyridazine (0.5 g, 3.46 mmol), dissolved in ethyl-methylketone was refluxed for 30 min. The unreacted ethyl-methylketone was distilled off yielding the crude material. The product was re-crystallized in alcohol to affoard colorless needles of (I).

### S3. Refinement

The H-atoms were positioned geometrically (N–H = 0.86, C–H = 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with $U_{iso}$(H) = x$U_{eq}$(C, N), where x = 1.5 for methyl and x = 1.2 for all other H-atoms.

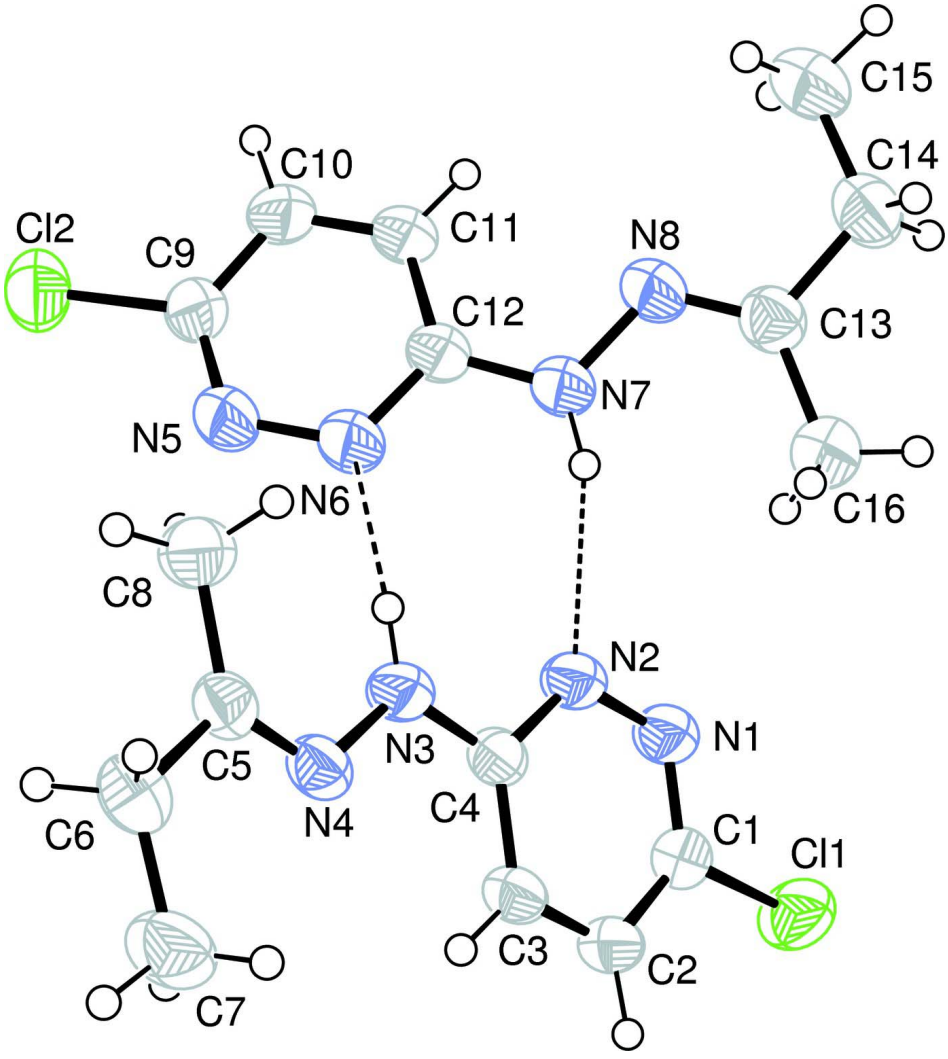


**Figure 1**

Two independent molecules of (I) with 50% probability displacement ellipsoids. Dashed lines denote intermolecular hydrogen bonds, forming a dimer: the N6 moleucle shown is generated by the symmetry operation (1–x, 1–y, –z) from the asymmetric atoms.

**3-[(2*E*)-2-(Butan-2-ylidene)hydrazinyl]-6-chloropyridazine**

*Crystal data*

$C_8H_{11}ClN_4$
$M_r = 198.66$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.0623\ (4)$ Å
$b = 11.6768\ (5)$ Å
$c = 12.1314\ (5)$ Å
$\alpha = 113.858\ (1)°$
$\beta = 91.370\ (2)°$
$\gamma = 104.880\ (2)°$
$V = 998.85\ (8)$ Å$^3$
$Z = 4$
$F(000) = 416$
$D_x = 1.321$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2652 reflections
$\theta = 2.1–25.3°$
$\mu = 0.34$ mm$^{-1}$
$T = 296$ K
Needle, colorless
0.25 × 0.15 × 0.14 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.10 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.982, $T_{max}$ = 0.988

14983 measured reflections
3585 independent reflections
2652 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031
$\theta_{max}$ = 25.3°, $\theta_{min}$ = 2.1°
$h$ = −9→9
$k$ = −13→13
$l$ = −14→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
$S$ = 1.05
3585 reflections
239 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
$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.1867P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.56878 (7) | 1.01144 (5) | 0.14461 (4) | 0.0711 (2) |
| N1 | 0.65078 (7) | 0.81818 (4) | −0.01826 (4) | 0.0494 (5) |
| N2 | 0.69138 (9) | 0.70411 (6) | −0.06328 (4) | 0.0477 (5) |
| N3 | 0.73568 (11) | 0.52631 (8) | −0.04789 (4) | 0.0485 (5) |
| N4 | 0.75811 (18) | 0.46292 (14) | 0.02371 (12) | 0.0446 (5) |
| C1 | 0.6218 (2) | 0.86549 (17) | 0.09480 (15) | 0.0457 (6) |
| C2 | 0.6309 (2) | 0.80724 (18) | 0.17388 (15) | 0.0482 (6) |
| C3 | 0.6692 (2) | 0.69257 (17) | 0.12939 (14) | 0.0456 (6) |
| C4 | 0.6972 (2) | 0.64155 (16) | 0.00695 (14) | 0.0403 (6) |
| C5 | 0.8018 (2) | 0.35764 (18) | −0.02463 (16) | 0.0446 (6) |
| C6 | 0.8294 (3) | 0.29374 (19) | 0.05683 (17) | 0.0546 (7) |
| C7 | 0.8037 (3) | 0.3631 (2) | 0.18693 (18) | 0.0706 (9) |
| C8 | 0.8324 (3) | 0.29472 (19) | −0.15401 (16) | 0.0571 (7) |
| Cl2 | 0.61890 (8) | 0.92216 (5) | 0.55956 (5) | 0.0741 (2) |
| N5 | 0.4684 (2) | 0.70148 (16) | 0.37821 (14) | 0.0577 (6) |
| N6 | 0.3743 (2) | 0.57428 (16) | 0.32230 (13) | 0.0577 (6) |
| N7 | 0.2290 (2) | 0.38112 (15) | 0.32596 (13) | 0.0557 (6) |

| | | | | |
|---|---|---|---|---|
| N8 | 0.1391 (2) | 0.31693 (16) | 0.38987 (13) | 0.0527 (6) |
| C9 | 0.4960 (2) | 0.75931 (18) | 0.49629 (16) | 0.0499 (6) |
| C10 | 0.4326 (3) | 0.69965 (19) | 0.57130 (16) | 0.0572 (7) |
| C11 | 0.3386 (3) | 0.57264 (19) | 0.51703 (16) | 0.0560 (7) |
| C12 | 0.3135 (2) | 0.51037 (18) | 0.38917 (15) | 0.0461 (6) |
| C13 | 0.0646 (3) | 0.19453 (19) | 0.33475 (16) | 0.0514 (7) |
| C14 | −0.0380 (3) | 0.1305 (2) | 0.40720 (18) | 0.0656 (8) |
| C15 | −0.0180 (3) | 0.2152 (2) | 0.5419 (2) | 0.0842 (10) |
| C16 | 0.06718 (9) | 0.10973 (7) | 0.20380 (5) | 0.0690 (8) |
| H2 | 0.61145 | 0.84592 | 0.25415 | 0.0578* |
| H3 | 0.67676 | 0.64881 | 0.17770 | 0.0547* |
| H3A | 0.74569 | 0.49409 | −0.12405 | 0.0582* |
| H6A | 0.75051 | 0.20566 | 0.02287 | 0.0655* |
| H6B | 0.94655 | 0.28638 | 0.05598 | 0.0655* |
| H7A | 0.88583 | 0.44865 | 0.22347 | 0.1059* |
| H7B | 0.68809 | 0.37098 | 0.18942 | 0.1059* |
| H7C | 0.82074 | 0.31382 | 0.23104 | 0.1059* |
| H8A | 0.72987 | 0.27583 | −0.20780 | 0.0858* |
| H8B | 0.92751 | 0.35314 | −0.16869 | 0.0858* |
| H8C | 0.85936 | 0.21485 | −0.16845 | 0.0858* |
| H7 | 0.23145 | 0.34080 | 0.24923 | 0.0668* |
| H10 | 0.45400 | 0.74553 | 0.65567 | 0.0687* |
| H11 | 0.29214 | 0.52778 | 0.56265 | 0.0673* |
| H14A | −0.00369 | 0.05316 | 0.39609 | 0.0787* |
| H14B | −0.15974 | 0.10162 | 0.37404 | 0.0787* |
| H15A | 0.10043 | 0.23887 | 0.57731 | 0.1264* |
| H15B | −0.09207 | 0.16776 | 0.57958 | 0.1264* |
| H15C | −0.04957 | 0.29300 | 0.55442 | 0.1264* |
| H16A | −0.00022 | 0.13112 | 0.15265 | 0.1035* |
| H16B | 0.01880 | 0.01944 | 0.18790 | 0.1035* |
| H16C | 0.18459 | 0.12428 | 0.18693 | 0.1035* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.1018 (5) | 0.0565 (3) | 0.0605 (3) | 0.0378 (3) | 0.0197 (3) | 0.0210 (3) |
| N1 | 0.0617 (10) | 0.0490 (9) | 0.0437 (8) | 0.0192 (8) | 0.0131 (7) | 0.0235 (7) |
| N2 | 0.0627 (10) | 0.0477 (9) | 0.0393 (8) | 0.0201 (8) | 0.0144 (7) | 0.0222 (7) |
| N3 | 0.0670 (10) | 0.0479 (9) | 0.0362 (7) | 0.0190 (8) | 0.0112 (7) | 0.0219 (7) |
| N4 | 0.0485 (9) | 0.0478 (9) | 0.0427 (8) | 0.0109 (7) | 0.0063 (7) | 0.0261 (7) |
| C1 | 0.0480 (11) | 0.0428 (10) | 0.0437 (10) | 0.0106 (8) | 0.0075 (8) | 0.0173 (8) |
| C2 | 0.0534 (11) | 0.0505 (11) | 0.0360 (9) | 0.0100 (9) | 0.0095 (8) | 0.0167 (8) |
| C3 | 0.0521 (11) | 0.0494 (11) | 0.0367 (9) | 0.0091 (9) | 0.0078 (8) | 0.0230 (8) |
| C4 | 0.0404 (10) | 0.0420 (10) | 0.0373 (9) | 0.0066 (8) | 0.0055 (7) | 0.0188 (8) |
| C5 | 0.0414 (10) | 0.0454 (11) | 0.0467 (10) | 0.0070 (8) | 0.0060 (8) | 0.0228 (9) |
| C6 | 0.0529 (12) | 0.0582 (12) | 0.0621 (12) | 0.0144 (10) | 0.0074 (9) | 0.0358 (10) |
| C7 | 0.0867 (16) | 0.0831 (16) | 0.0590 (12) | 0.0271 (13) | 0.0127 (11) | 0.0454 (12) |
| C8 | 0.0663 (13) | 0.0581 (12) | 0.0506 (11) | 0.0227 (10) | 0.0131 (9) | 0.0236 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Cl2 | 0.0911 (4) | 0.0514 (3) | 0.0707 (4) | 0.0066 (3) | 0.0057 (3) | 0.0259 (3) |
| N5 | 0.0740 (12) | 0.0536 (10) | 0.0461 (9) | 0.0099 (9) | 0.0093 (8) | 0.0269 (8) |
| N6 | 0.0790 (12) | 0.0537 (10) | 0.0401 (8) | 0.0104 (9) | 0.0088 (8) | 0.0249 (8) |
| N7 | 0.0760 (11) | 0.0497 (10) | 0.0379 (8) | 0.0079 (8) | 0.0112 (8) | 0.0213 (7) |
| N8 | 0.0610 (10) | 0.0546 (10) | 0.0466 (9) | 0.0123 (8) | 0.0115 (7) | 0.0282 (8) |
| C9 | 0.0580 (12) | 0.0459 (11) | 0.0482 (10) | 0.0162 (9) | 0.0093 (9) | 0.0215 (9) |
| C10 | 0.0795 (14) | 0.0535 (13) | 0.0373 (10) | 0.0183 (11) | 0.0123 (9) | 0.0185 (9) |
| C11 | 0.0786 (14) | 0.0534 (12) | 0.0409 (10) | 0.0169 (11) | 0.0182 (9) | 0.0256 (9) |
| C12 | 0.0540 (11) | 0.0488 (11) | 0.0394 (9) | 0.0147 (9) | 0.0086 (8) | 0.0225 (9) |
| C13 | 0.0534 (12) | 0.0540 (12) | 0.0493 (10) | 0.0128 (10) | 0.0069 (9) | 0.0261 (10) |
| C14 | 0.0692 (14) | 0.0642 (14) | 0.0642 (13) | 0.0077 (11) | 0.0132 (10) | 0.0349 (11) |
| C15 | 0.1004 (19) | 0.0848 (18) | 0.0671 (15) | 0.0104 (14) | 0.0291 (13) | 0.0410 (13) |
| C16 | 0.0818 (16) | 0.0572 (13) | 0.0572 (12) | 0.0078 (11) | 0.0125 (11) | 0.0212 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C1 | 1.734 (2) | C6—H6B | 0.9700 |
| Cl2—C9 | 1.733 (2) | C6—H6A | 0.9700 |
| N1—N2 | 1.3504 (9) | C7—H7A | 0.9600 |
| N1—C1 | 1.3075 (17) | C7—H7C | 0.9600 |
| N2—C4 | 1.3345 (19) | C7—H7B | 0.9600 |
| N3—N4 | 1.3843 (18) | C8—H8A | 0.9600 |
| N3—C4 | 1.360 (2) | C8—H8C | 0.9600 |
| N4—C5 | 1.276 (3) | C8—H8B | 0.9600 |
| N3—H3A | 0.8600 | C9—C10 | 1.388 (3) |
| N5—C9 | 1.297 (2) | C10—C11 | 1.348 (3) |
| N5—N6 | 1.350 (3) | C11—C12 | 1.405 (2) |
| N6—C12 | 1.333 (3) | C13—C16 | 1.4981 (19) |
| N7—N8 | 1.381 (2) | C13—C14 | 1.505 (3) |
| N7—C12 | 1.357 (3) | C14—C15 | 1.508 (3) |
| N8—C13 | 1.272 (3) | C10—H10 | 0.9300 |
| N7—H7 | 0.8600 | C11—H11 | 0.9300 |
| C1—C2 | 1.392 (3) | C14—H14A | 0.9700 |
| C2—C3 | 1.347 (3) | C14—H14B | 0.9700 |
| C3—C4 | 1.408 (2) | C15—H15A | 0.9600 |
| C5—C8 | 1.498 (3) | C15—H15B | 0.9600 |
| C5—C6 | 1.501 (3) | C15—H15C | 0.9600 |
| C6—C7 | 1.503 (3) | C16—H16A | 0.9600 |
| C2—H2 | 0.9300 | C16—H16B | 0.9600 |
| C3—H3 | 0.9300 | C16—H16C | 0.9600 |
| | | | |
| N2—N1—C1 | 118.43 (10) | H8A—C8—H8C | 109.00 |
| N1—N2—C4 | 119.67 (8) | C5—C8—H8A | 109.00 |
| N4—N3—C4 | 117.38 (10) | H8B—C8—H8C | 109.00 |
| N3—N4—C5 | 118.39 (13) | H8A—C8—H8B | 109.00 |
| C4—N3—H3A | 121.00 | C5—C8—H8C | 109.00 |
| N4—N3—H3A | 121.00 | C5—C8—H8B | 109.00 |
| N6—N5—C9 | 119.09 (18) | Cl2—C9—C10 | 119.98 (14) |

| | | | |
|---|---|---|---|
| N5—N6—C12 | 119.53 (15) | Cl2—C9—N5 | 115.69 (16) |
| N8—N7—C12 | 117.28 (14) | N5—C9—C10 | 124.3 (2) |
| N7—N8—C13 | 119.01 (15) | C9—C10—C11 | 117.37 (17) |
| N8—N7—H7 | 121.00 | C10—C11—C12 | 117.67 (19) |
| C12—N7—H7 | 121.00 | N7—C12—C11 | 122.28 (19) |
| N1—C1—C2 | 124.75 (16) | N6—C12—N7 | 115.75 (15) |
| Cl1—C1—C2 | 119.92 (13) | N6—C12—C11 | 121.96 (19) |
| Cl1—C1—N1 | 115.33 (13) | N8—C13—C14 | 116.84 (17) |
| C1—C2—C3 | 117.28 (16) | N8—C13—C16 | 125.68 (18) |
| C2—C3—C4 | 117.42 (17) | C14—C13—C16 | 117.47 (17) |
| N2—C4—N3 | 114.99 (12) | C13—C14—C15 | 115.48 (19) |
| N3—C4—C3 | 122.59 (16) | C9—C10—H10 | 121.00 |
| N2—C4—C3 | 122.41 (16) | C11—C10—H10 | 121.00 |
| C6—C5—C8 | 117.44 (18) | C10—C11—H11 | 121.00 |
| N4—C5—C8 | 125.76 (19) | C12—C11—H11 | 121.00 |
| N4—C5—C6 | 116.78 (16) | C13—C14—H14A | 108.00 |
| C5—C6—C7 | 115.54 (19) | C13—C14—H14B | 108.00 |
| C3—C2—H2 | 121.00 | C15—C14—H14A | 108.00 |
| C1—C2—H2 | 121.00 | C15—C14—H14B | 108.00 |
| C4—C3—H3 | 121.00 | H14A—C14—H14B | 107.00 |
| C2—C3—H3 | 121.00 | C14—C15—H15A | 109.00 |
| C5—C6—H6A | 108.00 | C14—C15—H15B | 109.00 |
| C7—C6—H6B | 108.00 | C14—C15—H15C | 109.00 |
| C5—C6—H6B | 108.00 | H15A—C15—H15B | 110.00 |
| H6A—C6—H6B | 107.00 | H15A—C15—H15C | 109.00 |
| C7—C6—H6A | 108.00 | H15B—C15—H15C | 110.00 |
| H7A—C7—H7B | 110.00 | C13—C16—H16A | 109.00 |
| H7A—C7—H7C | 109.00 | C13—C16—H16B | 109.00 |
| C6—C7—H7C | 109.00 | C13—C16—H16C | 109.00 |
| H7B—C7—H7C | 109.00 | H16A—C16—H16B | 109.00 |
| C6—C7—H7B | 109.00 | H16A—C16—H16C | 109.00 |
| C6—C7—H7A | 109.00 | H16B—C16—H16C | 109.00 |

| | | | |
|---|---|---|---|
| C1—N1—N2—C4 | 1.45 (15) | N8—N7—C12—C11 | 12.0 (3) |
| N2—N1—C1—Cl1 | −179.47 (8) | N7—N8—C13—C16 | 1.2 (3) |
| N2—N1—C1—C2 | 0.5 (2) | N7—N8—C13—C14 | −177.43 (18) |
| N1—N2—C4—N3 | 178.67 (10) | N1—C1—C2—C3 | −1.3 (3) |
| N1—N2—C4—C3 | −2.6 (2) | Cl1—C1—C2—C3 | 178.68 (14) |
| C4—N3—N4—C5 | −176.95 (15) | C1—C2—C3—C4 | 0.2 (3) |
| N4—N3—C4—N2 | 174.58 (12) | C2—C3—C4—N2 | 1.8 (3) |
| N4—N3—C4—C3 | −4.1 (2) | C2—C3—C4—N3 | −179.62 (16) |
| N3—N4—C5—C6 | 178.44 (15) | N4—C5—C6—C7 | −0.6 (3) |
| N3—N4—C5—C8 | 0.2 (3) | C8—C5—C6—C7 | 177.78 (19) |
| C9—N5—N6—C12 | −0.8 (3) | Cl2—C9—C10—C11 | −179.66 (18) |
| N6—N5—C9—Cl2 | 179.70 (14) | N5—C9—C10—C11 | 1.1 (3) |
| N6—N5—C9—C10 | −1.0 (3) | C9—C10—C11—C12 | 0.6 (3) |
| N5—N6—C12—N7 | −176.31 (16) | C10—C11—C12—N6 | −2.3 (3) |
| N5—N6—C12—C11 | 2.5 (3) | C10—C11—C12—N7 | 176.4 (2) |

| | | | |
|---|---|---|---|
| C12—N7—N8—C13 | −176.99 (19) | N8—C13—C14—C15 | −8.9 (3) |
| N8—N7—C12—N6 | −169.24 (16) | C16—C13—C14—C15 | 172.35 (18) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*A*···N6$^{i}$ | 0.86 | 2.30 | 3.0674 (15) | 148 |
| N7—H7···N2$^{i}$ | 0.86 | 2.24 | 3.0689 (15) | 161 |

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