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# 6,6′-Dinitro-1,1′-(ethane-1,2-diyl)di(1*H*-indazole)

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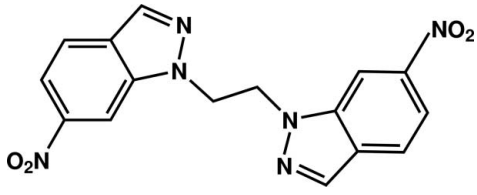
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.039; $wR$ factor = 0.111; data-to-parameter ratio = 14.8.

The molecule of the title compound, $C_{16}H_{12}N_6O_4$, is built up from two fused five- and six-membered rings linked by an ethylene group. The dihedral angle between the planes through the indazole ring systems is 39.74 (5)°. The nitro groups are tilted by 7.2 (2) and 8.5 (2)° with respect to planes of the fused-ring systems. In the crystal, molecules are linked by C—H···N and C—H···O hydrogen bonds into chains running parallel to the $c$ axis.

## Related literature

For biological activities of the indazole moiety, see: Ali *et al.* (2012); Abbassi *et al.* (2012); Plescia *et al.* (2010); Lee *et al.* (2001); Liu *et al.* (2011). For related compounds, see: Kouakou *et al.* (2013); Chicha *et al.* (2013).




## Experimental

### Crystal data

$C_{16}H_{12}N_6O_4$
$M_r$ = 352.32
Monoclinic, $P2_1/c$
$a$ = 9.410 (5) Å
$b$ = 12.064 (5) Å
$c$ = 14.804 (4) Å
$\beta$ = 109.01 (2)°
$V$ = 1588.9 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 296 K
0.37 × 0.32 × 0.26 mm

### Data collection

Bruker X8 APEX diffractometer
16446 measured reflections
3503 independent reflections
2667 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
$S$ = 1.03
3503 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C7—H7···N5$^{i}$ | 0.93 | 2.48 | 3.344 (2) | 154 |
| C15—H15···O1$^{i}$ | 0.93 | 2.47 | 3.401 (2) | 179 |

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

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, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: RZ5107).

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# supporting information

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## 6,6′-Dinitro-1,1′-(ethane-1,2-diyl)di(1*H*-indazole)

**Assoman Kouakou, El Mostapha Rakib, Abdelghani El Malki, Mohamed Saadi and Lahcen El Ammari**

### S1. Comment

Indazole moiety have been nucleus is a pharmaceutically important and emerging heterocycle with a broad spectrum of activities including anti-microbial1, anti-cancer, anti-inflammatory, anti- platelet, and selective 5-HT6 antagonists (Ali *et al.*, 2012; Abbassi *et al.*, 2012; Plescia *et al.*, 2010; Lee *et al.*, 2001; Liu *et al.*, 2011). The present work is a continuation of the investigation on the indazole derivatives published recently by our team (Kouakou *et al.*, 2013; Chicha *et al.*, 2013).

The molecule of the title compound is formed by two fused five- and six-membered rings linked by an ethylene group and connected to two nitro groups as shown in Fig. 1. The two fused ring systems (N2/N3/C1–C7 and N4/N5C10–C16) make dihedral angles of 7.2 (2)° and 8.5 (2)° with the planes through the attached nitro groups (N1/O1/O2 and N6/O3(O4), respectively. The dihedral angle between the indazole ring systems is 39.74 (5)°. In the crystal, molecules are linked by C7—H7···N5 and C15—H15···O1 hydrogen interactions (Table 1) into chains running parallel to the [0 0 1] direction as shown in Fig. 2.

### S2. Experimental

A solution of 6-nitroindazole (0.5 g, 3.06 mmol) and KOH (0.17 g, 3.08 mmol) in EtOH (15 ml) was heated under reflux for 48 h. The mixture was cooled and the solvent removed from the filtrate *in vacuo*. The formed 6-nitroindazole potassium salt and 1,2-ethylene dibromide (0.27 ml, 1.48 mmol) was heated in dimethylformamide (5 ml) under reflux for 3 h. The mixture was then cooled, all volatiles were removed *in vacuo* and water was added. The precipitate was filtered and was purified by column chromatography (EtOAc/hexane 2:8 *v*/*v*). The title compound was recrystallized from acetone (yield: 35%; m. p.: 468 K).

### S3. Refinement

H atoms were located in a difference Fourier map and treated as riding, with C–H = 0.93-0.97 Å and with $U_{iso}$(H) = 1.2 $U_{eq}$(C). One outlier (0 1 1) was omitted in the last cycles of refinement.

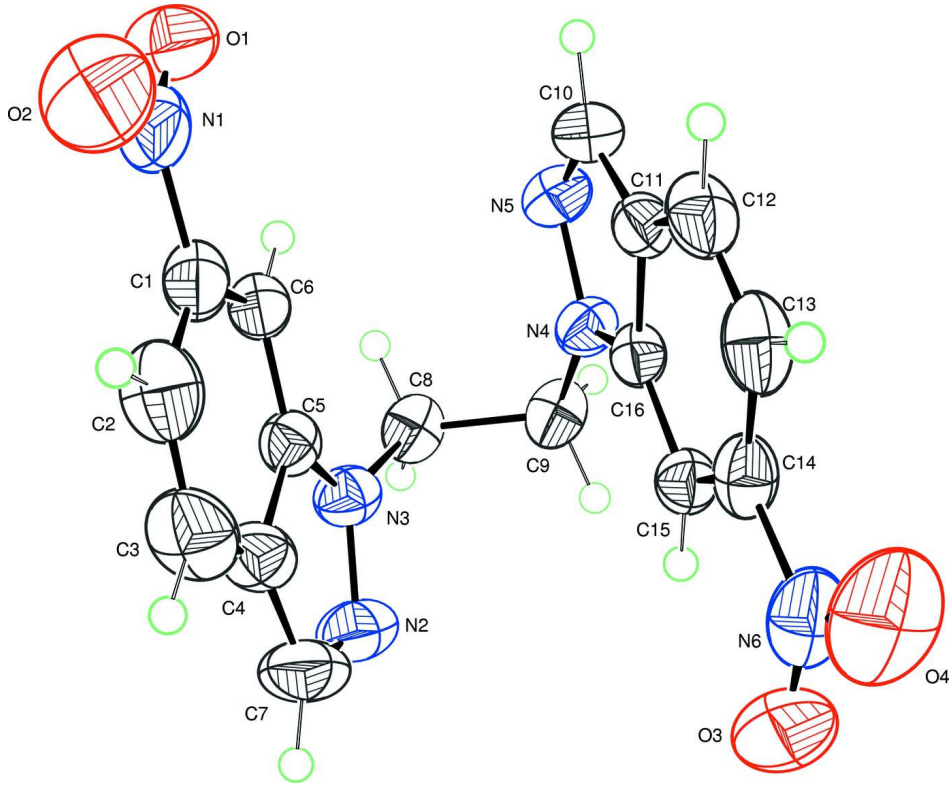


**Figure 1**

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are represented as small circles.

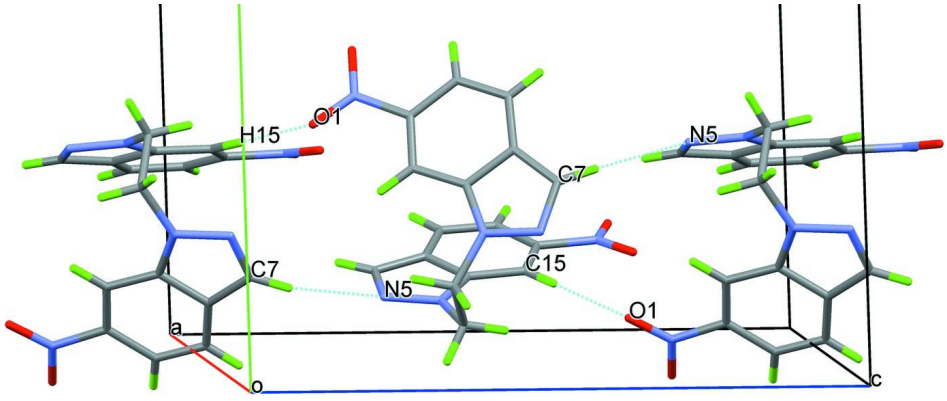


**Figure 2**

Partial crystal packing of the title compound showing a chain of molecules linked by hydrogen bonds (dashed lines).

### 6,6′-Dinitro-1,1′-(ethane-1,2-diyl)di(1*H*-indazole)

*Crystal data*

$C_{16}H_{12}N_6O_4$
$M_r$ = 352.32
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 9.410 (5) Å
$b$ = 12.064 (5) Å
$c$ = 14.804 (4) Å
$\beta$ = 109.01 (2)°
$V$ = 1588.9 (12) Å$^3$
$Z$ = 4

$F(000) = 728$
$D_x = 1.473$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3672 reflections
$\theta = 1.5–27.1°$
$\mu = 0.11$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.37 × 0.32 × 0.26 mm

*Data collection*

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
16446 measured reflections
3503 independent reflections
2667 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.1°$, $\theta_{min} = 2.8°$
$h = -12 \rightarrow 12$
$k = -15 \rightarrow 15$
$l = -18 \rightarrow 18$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.111$
$S = 1.03$
3503 reflections
236 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
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.3594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å$^{-3}$
$\Delta\rho_{min} = -0.19$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0033 (10)

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.72668 (16) | 0.44512 (14) | 0.20575 (10) | 0.0753 (4) |
| O2 | 0.8642 (2) | 0.57503 (14) | 0.28985 (14) | 0.1037 (6) |
| O3 | 1.06798 (18) | 0.14604 (14) | 0.75890 (9) | 0.0817 (5) |
| O4 | 1.28535 (16) | 0.17800 (15) | 0.74730 (11) | 0.0990 (6) |
| N1 | 0.78171 (17) | 0.49484 (13) | 0.28105 (13) | 0.0617 (4) |
| N2 | 0.53003 (16) | 0.25102 (14) | 0.54188 (9) | 0.0580 (4) |
| N3 | 0.54014 (13) | 0.24766 (11) | 0.45233 (8) | 0.0435 (3) |
| N4 | 0.74940 (12) | 0.09097 (10) | 0.40649 (8) | 0.0384 (3) |
| N5 | 0.74567 (15) | 0.09998 (12) | 0.31430 (8) | 0.0487 (3) |
| N6 | 1.15060 (18) | 0.16124 (12) | 0.71175 (11) | 0.0612 (4) |
| C1 | 0.74301 (17) | 0.45822 (13) | 0.36515 (12) | 0.0474 (4) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.7928 (2) | 0.52228 (15) | 0.44873 (15) | 0.0630 (5) |
| H2 | 0.8535 | 0.5839 | 0.4515 | 0.076* |
| C3 | 0.7517 (2) | 0.49382 (17) | 0.52569 (14) | 0.0669 (5) |
| H3 | 0.7817 | 0.5367 | 0.5809 | 0.080* |
| C4 | 0.66362 (18) | 0.39900 (15) | 0.52037 (11) | 0.0504 (4) |
| C5 | 0.62089 (15) | 0.33505 (12) | 0.43641 (10) | 0.0386 (3) |
| C6 | 0.65760 (16) | 0.36455 (12) | 0.35590 (10) | 0.0407 (3) |
| H6 | 0.6263 | 0.3234 | 0.2997 | 0.049* |
| C7 | 0.6008 (2) | 0.34107 (18) | 0.58152 (12) | 0.0645 (5) |
| H7 | 0.6090 | 0.3644 | 0.6429 | 0.077* |
| C8 | 0.49431 (15) | 0.14827 (13) | 0.39587 (11) | 0.0439 (4) |
| H8A | 0.4747 | 0.1659 | 0.3290 | 0.053* |
| H8B | 0.4017 | 0.1208 | 0.4030 | 0.053* |
| C9 | 0.61375 (15) | 0.05839 (13) | 0.42568 (11) | 0.0443 (4) |
| H9A | 0.6375 | 0.0436 | 0.4934 | 0.053* |
| H9B | 0.5748 | −0.0094 | 0.3912 | 0.053* |
| C10 | 0.87881 (19) | 0.13663 (14) | 0.31726 (11) | 0.0505 (4) |
| H10 | 0.9067 | 0.1501 | 0.2635 | 0.061* |
| C11 | 0.97408 (16) | 0.15298 (12) | 0.41201 (10) | 0.0401 (3) |
| C12 | 1.12332 (17) | 0.18656 (13) | 0.45625 (13) | 0.0511 (4) |
| H12 | 1.1830 | 0.2074 | 0.4199 | 0.061* |
| C13 | 1.17921 (16) | 0.18815 (13) | 0.55331 (13) | 0.0520 (4) |
| H13 | 1.2785 | 0.2087 | 0.5841 | 0.062* |
| C14 | 1.08659 (16) | 0.15870 (12) | 0.60685 (11) | 0.0433 (4) |
| C15 | 0.93939 (15) | 0.12611 (12) | 0.56797 (10) | 0.0375 (3) |
| H15 | 0.8802 | 0.1076 | 0.6052 | 0.045* |
| C16 | 0.88544 (14) | 0.12277 (11) | 0.46851 (9) | 0.0337 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0816 (9) | 0.0892 (11) | 0.0650 (9) | 0.0071 (8) | 0.0377 (7) | 0.0152 (8) |
| O2 | 0.1124 (13) | 0.0726 (11) | 0.1501 (16) | −0.0232 (10) | 0.0756 (12) | 0.0175 (10) |
| O3 | 0.0884 (10) | 0.1023 (12) | 0.0437 (7) | 0.0028 (9) | 0.0066 (7) | −0.0094 (7) |
| O4 | 0.0647 (9) | 0.1077 (13) | 0.0874 (11) | −0.0184 (8) | −0.0262 (8) | −0.0118 (9) |
| N1 | 0.0585 (9) | 0.0505 (9) | 0.0863 (12) | 0.0087 (7) | 0.0376 (8) | 0.0203 (8) |
| N2 | 0.0521 (8) | 0.0823 (11) | 0.0423 (8) | 0.0015 (8) | 0.0193 (6) | 0.0077 (7) |
| N3 | 0.0397 (6) | 0.0518 (8) | 0.0396 (7) | −0.0015 (6) | 0.0139 (5) | 0.0034 (5) |
| N4 | 0.0345 (6) | 0.0445 (7) | 0.0350 (6) | −0.0009 (5) | 0.0096 (5) | 0.0047 (5) |
| N5 | 0.0539 (8) | 0.0556 (8) | 0.0348 (7) | 0.0022 (6) | 0.0122 (5) | 0.0045 (6) |
| N6 | 0.0602 (9) | 0.0482 (9) | 0.0565 (9) | −0.0003 (7) | −0.0065 (7) | −0.0092 (7) |
| C1 | 0.0448 (8) | 0.0398 (9) | 0.0594 (10) | 0.0049 (7) | 0.0195 (7) | 0.0067 (7) |
| C2 | 0.0607 (11) | 0.0428 (10) | 0.0824 (13) | −0.0098 (8) | 0.0189 (9) | −0.0067 (9) |
| C3 | 0.0704 (12) | 0.0604 (12) | 0.0614 (12) | −0.0067 (9) | 0.0098 (9) | −0.0233 (9) |
| C4 | 0.0484 (8) | 0.0589 (11) | 0.0403 (8) | 0.0030 (8) | 0.0096 (7) | −0.0072 (7) |
| C5 | 0.0340 (7) | 0.0411 (8) | 0.0386 (7) | 0.0026 (6) | 0.0088 (6) | 0.0006 (6) |
| C6 | 0.0425 (8) | 0.0388 (8) | 0.0402 (8) | 0.0044 (6) | 0.0126 (6) | 0.0003 (6) |
| C7 | 0.0645 (11) | 0.0929 (15) | 0.0362 (9) | 0.0050 (10) | 0.0164 (8) | −0.0053 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0307 (7) | 0.0476 (9) | 0.0490 (8) | −0.0051 (6) | 0.0068 (6) | 0.0043 (7) |
| C9 | 0.0341 (7) | 0.0446 (9) | 0.0510 (9) | −0.0058 (6) | 0.0095 (6) | 0.0098 (7) |
| C10 | 0.0589 (10) | 0.0556 (10) | 0.0445 (9) | 0.0084 (8) | 0.0272 (7) | 0.0085 (7) |
| C11 | 0.0410 (7) | 0.0369 (8) | 0.0481 (8) | 0.0058 (6) | 0.0221 (6) | 0.0066 (6) |
| C12 | 0.0387 (8) | 0.0456 (9) | 0.0772 (12) | 0.0017 (7) | 0.0300 (8) | 0.0100 (8) |
| C13 | 0.0307 (7) | 0.0395 (9) | 0.0805 (12) | −0.0024 (6) | 0.0110 (7) | 0.0025 (8) |
| C14 | 0.0396 (7) | 0.0328 (8) | 0.0494 (9) | 0.0009 (6) | 0.0035 (6) | −0.0035 (6) |
| C15 | 0.0376 (7) | 0.0354 (7) | 0.0399 (7) | 0.0015 (6) | 0.0132 (6) | 0.0017 (6) |
| C16 | 0.0304 (6) | 0.0311 (7) | 0.0397 (7) | 0.0020 (5) | 0.0117 (5) | 0.0027 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—N1 | 1.223 (2) | C4—C7 | 1.416 (3) |
| O2—N1 | 1.220 (2) | C5—C6 | 1.391 (2) |
| O3—N6 | 1.216 (2) | C6—H6 | 0.9300 |
| O4—N6 | 1.221 (2) | C7—H7 | 0.9300 |
| N1—C1 | 1.474 (2) | C8—C9 | 1.520 (2) |
| N2—C7 | 1.309 (3) | C8—H8A | 0.9700 |
| N2—N3 | 1.3603 (18) | C8—H8B | 0.9700 |
| N3—C5 | 1.3643 (19) | C9—H9A | 0.9700 |
| N3—C8 | 1.445 (2) | C9—H9B | 0.9700 |
| N4—N5 | 1.3581 (17) | C10—C11 | 1.411 (2) |
| N4—C16 | 1.3650 (18) | C10—H10 | 0.9300 |
| N4—C9 | 1.4494 (19) | C11—C12 | 1.402 (2) |
| N5—C10 | 1.316 (2) | C11—C16 | 1.4082 (19) |
| N6—C14 | 1.472 (2) | C12—C13 | 1.360 (2) |
| C1—C6 | 1.367 (2) | C12—H12 | 0.9300 |
| C1—C2 | 1.404 (2) | C13—C14 | 1.401 (2) |
| C2—C3 | 1.361 (3) | C13—H13 | 0.9300 |
| C2—H2 | 0.9300 | C14—C15 | 1.373 (2) |
| C3—C4 | 1.400 (3) | C15—C16 | 1.3929 (19) |
| C3—H3 | 0.9300 | C15—H15 | 0.9300 |
| C4—C5 | 1.406 (2) | | |

| | | | |
|---|---|---|---|
| O2—N1—O1 | 123.51 (18) | C4—C7—H7 | 123.8 |
| O2—N1—C1 | 118.09 (18) | N3—C8—C9 | 111.77 (12) |
| O1—N1—C1 | 118.37 (15) | N3—C8—H8A | 109.3 |
| C7—N2—N3 | 105.94 (14) | C9—C8—H8A | 109.3 |
| N2—N3—C5 | 111.41 (13) | N3—C8—H8B | 109.3 |
| N2—N3—C8 | 119.09 (13) | C9—C8—H8B | 109.3 |
| C5—N3—C8 | 128.28 (12) | H8A—C8—H8B | 107.9 |
| N5—N4—C16 | 111.41 (11) | N4—C9—C8 | 111.39 (12) |
| N5—N4—C9 | 118.85 (11) | N4—C9—H9A | 109.3 |
| C16—N4—C9 | 129.58 (12) | C8—C9—H9A | 109.3 |
| C10—N5—N4 | 106.31 (12) | N4—C9—H9B | 109.3 |
| O3—N6—O4 | 123.09 (18) | C8—C9—H9B | 109.3 |
| O3—N6—C14 | 118.95 (15) | H9A—C9—H9B | 108.0 |
| O4—N6—C14 | 117.96 (18) | N5—C10—C11 | 111.71 (13) |

| | | | |
|---|---|---|---|
| C6—C1—C2 | 124.04 (16) | N5—C10—H10 | 124.1 |
| C6—C1—N1 | 117.51 (15) | C11—C10—H10 | 124.1 |
| C2—C1—N1 | 118.44 (16) | C12—C11—C16 | 119.62 (14) |
| C3—C2—C1 | 119.66 (17) | C12—C11—C10 | 136.07 (14) |
| C3—C2—H2 | 120.2 | C16—C11—C10 | 104.29 (13) |
| C1—C2—H2 | 120.2 | C13—C12—C11 | 118.78 (14) |
| C2—C3—C4 | 118.92 (16) | C13—C12—H12 | 120.6 |
| C2—C3—H3 | 120.5 | C11—C12—H12 | 120.6 |
| C4—C3—H3 | 120.5 | C12—C13—C14 | 119.75 (14) |
| C3—C4—C5 | 119.45 (16) | C12—C13—H13 | 120.1 |
| C3—C4—C7 | 136.90 (17) | C14—C13—H13 | 120.1 |
| C5—C4—C7 | 103.63 (16) | C15—C14—C13 | 124.32 (15) |
| N3—C5—C6 | 130.81 (13) | C15—C14—N6 | 117.30 (15) |
| N3—C5—C4 | 106.64 (13) | C13—C14—N6 | 118.38 (14) |
| C6—C5—C4 | 122.54 (15) | C14—C15—C16 | 114.97 (13) |
| C1—C6—C5 | 115.31 (14) | C14—C15—H15 | 122.5 |
| C1—C6—H6 | 122.3 | C16—C15—H15 | 122.5 |
| C5—C6—H6 | 122.3 | N4—C16—C15 | 131.16 (12) |
| N2—C7—C4 | 112.36 (15) | N4—C16—C11 | 106.28 (12) |
| N2—C7—H7 | 123.8 | C15—C16—C11 | 122.54 (13) |

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| C7—N2—N3—C5 | 1.38 (17) | C5—N3—C8—C9 | 87.72 (18) |
| C7—N2—N3—C8 | 169.77 (14) | N5—N4—C9—C8 | −68.45 (17) |
| C16—N4—N5—C10 | 0.40 (17) | C16—N4—C9—C8 | 106.61 (16) |
| C9—N4—N5—C10 | 176.31 (14) | N3—C8—C9—N4 | −65.19 (17) |
| O2—N1—C1—C6 | −176.34 (16) | N4—N5—C10—C11 | −0.10 (18) |
| O1—N1—C1—C6 | 5.4 (2) | N5—C10—C11—C12 | 177.90 (17) |
| O2—N1—C1—C2 | 5.0 (2) | N5—C10—C11—C16 | −0.21 (18) |
| O1—N1—C1—C2 | −173.22 (15) | C16—C11—C12—C13 | 0.6 (2) |
| C6—C1—C2—C3 | −2.2 (3) | C10—C11—C12—C13 | −177.33 (17) |
| N1—C1—C2—C3 | 176.39 (16) | C11—C12—C13—C14 | −1.3 (2) |
| C1—C2—C3—C4 | 1.7 (3) | C12—C13—C14—C15 | 0.8 (2) |
| C2—C3—C4—C5 | 0.6 (3) | C12—C13—C14—N6 | 179.97 (14) |
| C2—C3—C4—C7 | 178.7 (2) | O3—N6—C14—C15 | −7.5 (2) |
| N2—N3—C5—C6 | −179.39 (14) | O4—N6—C14—C15 | 172.00 (16) |
| C8—N3—C5—C6 | 13.6 (2) | O3—N6—C14—C13 | 173.18 (16) |
| N2—N3—C5—C4 | −0.72 (16) | O4—N6—C14—C13 | −7.3 (2) |
| C8—N3—C5—C4 | −167.77 (13) | C13—C14—C15—C16 | 0.6 (2) |
| C3—C4—C5—N3 | 178.52 (15) | N6—C14—C15—C16 | −178.62 (12) |
| C7—C4—C5—N3 | −0.18 (17) | N5—N4—C16—C15 | −179.32 (14) |
| C3—C4—C5—C6 | −2.7 (2) | C9—N4—C16—C15 | 5.3 (3) |
| C7—C4—C5—C6 | 178.62 (14) | N5—N4—C16—C11 | −0.53 (15) |
| C2—C1—C6—C5 | 0.2 (2) | C9—N4—C16—C11 | −175.88 (14) |
| N1—C1—C6—C5 | −178.41 (12) | C14—C15—C16—N4 | 177.23 (14) |
| N3—C5—C6—C1 | −179.27 (14) | C14—C15—C16—C11 | −1.4 (2) |
| C4—C5—C6—C1 | 2.2 (2) | C12—C11—C16—N4 | −178.06 (13) |
| N3—N2—C7—C4 | −1.5 (2) | C10—C11—C16—N4 | 0.43 (15) |
| C3—C4—C7—N2 | −177.3 (2) | C12—C11—C16—C15 | 0.9 (2) |

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| C5—C4—C7—N2 | 1.1 (2) | C10—C11—C16—C15 | 179.35 (13) |
| N2—N3—C8—C9 | −78.47 (16) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7···N5$^{i}$ | 0.93 | 2.48 | 3.344 (2) | 154 |
| C15—H15···O1$^{i}$ | 0.93 | 2.47 | 3.401 (2) | 179 |

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