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# 15a,15b-Dihydro-5*H*,7*H*,9*H*,14*H*,17*H*-15,16-methanodibenzo[e]diazepino-[2,3-c;3′,2′-e]imidazole-7,18-dione

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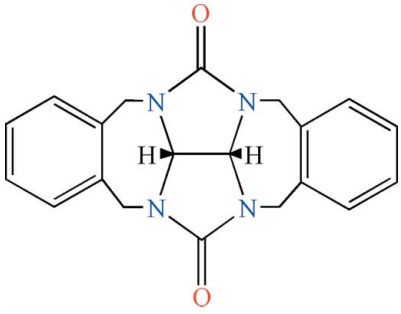
Key indicators: single-crystal X-ray study; $T$ = 292 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.053; $wR$ factor = 0.127; data-to-parameter ratio = 15.5.

The title compound, $C_{20}H_{18}N_4O_2$, is a molecular clip based on the glycoluril framework. The two benzene rings are each fused to a seven-membered ring; these rings bind four of the N atoms from separate rings of the glycoluril system to form the sidewalls of the molecular clip. The crystal packing is stabilized by non-classical C—H···O hydrogen bonds. There are no $\pi$–$\pi$ stacking interactions in the crystal structure. The molecule provides a model with approximate non-crystallographic $C_{2v}$ symmetry.

## Related literature

For the preparation of the title compound, see: Wang *et al.* (2006). For historical background of the title compound, see: Rowan *et al.* (1999); Yin *et al.* (2006); Li *et al.* (2006); Freeman *et al.* (1981); Rebek (2005); Wu *et al.* (2002).




## Experimental

### Crystal data

$C_{20}H_{18}N_4O_2$
$M_r$ = 346.38
Monoclinic, $P2_1/n$
$a$ = 10.2660 (16) Å
$b$ = 11.2985 (18) Å
$c$ = 14.522 (2) Å
$\beta$ = 97.923 (3)°
$V$ = 1668.3 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 292 (2) K
0.20 × 0.10 × 0.04 mm

### Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
13800 measured reflections
3632 independent reflections
2139 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.127
$S$ = 0.98
3632 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C19—H19···O1$^{i}$ | 0.93 | 2.55 | 3.252 (3) | 132 |
| C7—H7$A$···O2$^{ii}$ | 0.97 | 2.45 | 3.343 (3) | 153 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

We thank Dr Xiang-Gao Meng for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2040).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4480 [ **doi:10.1107/S1600536807053378** ]

# 15a,15b-Dihydro-5*H*,7*H*,9*H*,14*H*,17*H*-15,16-methanodibenzo[*e*]diazepino[2,3-*c*;3',2'-*e*]imidazole-7,18-dione

**Y. Hu, B. Zhou and L. Cao**

## Comment

The glycoluril skeleton has served as an important building block for the preparation of a wide variety of supramolecular systems, including molecular clips (Rowan *et al.*, 1999; Yin *et al.*, 2006; Li *et al.*, 2006), the cucurbit[*n*]uril family (Freeman *et al.*, 1981), and molecular capsules (Rebek,2005). In addition, Isaacs and co-workers have synthesized many methlene-bridged glycouril dimers from the title compound (Wu *et al.*, 2002).

The molecular structure of the title compound is shown in Fig. 1. The crystal packing is stabilized by inversion-related intermolecular C19—H19···O1 hydrogen bonds, forming dimers. These dimers are linked by additional C7—H7A···O2 hydrogen bonds (Table 1). Many examples of π···π interactions between the molecular clips are observed in the crystal structures presented by Wang *et al.* (2006), however, there are no such interactions observed in our example structure.

## Experimental

The title compound was synthesized according to the procedure of Wang *et al.* (2006) in 42% isolated yield. Crystals of the title compound suitable for X-ray data collection were obtained by slow evaporation of a chloroform and methaol solution in ratio of 100:1 at 293 K.

## Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined using a riding model, with $U_{iso}$(H) = 1.2 $U_{eq}$(C) (1.5$U_{eq}$(C) for methly) of the parent atoms.

## Figures

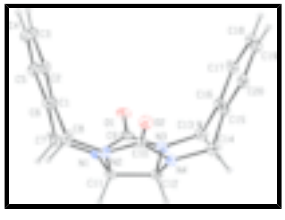

Fig. 1. View of the title molecule showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 10% probability level. H atoms are represented by spheres of arbitrary radius.

## 15a,15*b*-Dihydro-5H,7*H*,9H,14*H*,17*H*-15,16-methanodibenzo[e]diazepino\ [2,3 – c;3',2'-e]imidazole-7,18-dione

*Crystal data*

$C_{20}H_{18}N_4O_2$ $F_{000}$ = 728

| | |
|---|---|
| $M_r$ = 346.38 | $D_x$ = 1.379 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 1842 reflections |
| $a$ = 10.2660 (16) Å | θ = 2.3–20.2º |
| $b$ = 11.2985 (18) Å | μ = 0.09 mm$^{-1}$ |
| $c$ = 14.522 (2) Å | $T$ = 292 (2) K |
| β = 97.923 (3)º | Plate, colorless |
| $V$ = 1668.3 (4) Å$^3$ | 0.20 × 0.10 × 0.04 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART 4K CCD area-detector diffractometer | 2139 reflections with $I > 2\sigma(I)$' |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.056 |
| Monochromator: graphite | $\theta_{max}$ = 27.0º |
| $T$ = 292(2) K | $\theta_{min}$ = 2.3º |
| φ and ω scans | $h$ = −12→13 |
| Absorption correction: none | $k$ = −14→14 |
| 13800 measured reflections | $l$ = −18→18 |
| 3632 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.053 | H-atom parameters constrained |
| $wR(F^2)$ = 0.127 | $w = 1/[\sigma^2(F_o^2) + (0.054P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.98 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 3632 reflections | $\Delta\rho_{max}$ = 0.16 e Å$^{-3}$ |
| 235 parameters | $\Delta\rho_{min}$ = −0.16 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.09320 (19) | 0.78732 (18) | 0.33914 (14) | 0.0469 (5) |
| C2 | 0.0178 (2) | 0.6858 (2) | 0.32550 (18) | 0.0608 (6) |
| H2 | 0.0016 | 0.6526 | 0.2664 | 0.073* |
| C3 | −0.0341 (2) | 0.6327 (2) | 0.3985 (2) | 0.0768 (8) |
| H3 | −0.0834 | 0.5636 | 0.3887 | 0.092* |
| C4 | −0.0123 (2) | 0.6827 (3) | 0.4847 (2) | 0.0790 (8) |
| H4 | −0.0470 | 0.6479 | 0.5340 | 0.095* |
| C5 | 0.0606 (2) | 0.7841 (2) | 0.49881 (16) | 0.0645 (7) |
| H5 | 0.0733 | 0.8181 | 0.5577 | 0.077* |
| C6 | 0.11589 (19) | 0.83734 (18) | 0.42791 (14) | 0.0464 (5) |
| C7 | 0.1984 (2) | 0.94700 (19) | 0.44777 (15) | 0.0559 (6) |
| H7A | 0.1569 | 1.0117 | 0.4109 | 0.067* |
| H7B | 0.2004 | 0.9678 | 0.5127 | 0.067* |
| C8 | 0.1512 (2) | 0.8415 (2) | 0.25890 (14) | 0.0574 (6) |
| H8A | 0.1235 | 0.7954 | 0.2033 | 0.069* |
| H8B | 0.1165 | 0.9209 | 0.2482 | 0.069* |
| C9 | 0.4266 (2) | 0.87315 (16) | 0.48619 (14) | 0.0470 (5) |
| C10 | 0.3746 (2) | 0.76527 (19) | 0.24463 (13) | 0.0471 (5) |
| C11 | 0.3627 (2) | 0.93601 (17) | 0.33387 (13) | 0.0468 (5) |
| H11 | 0.3530 | 1.0153 | 0.3065 | 0.056* |
| C12 | 0.5054 (2) | 0.89188 (17) | 0.34320 (13) | 0.0476 (5) |
| H12 | 0.5668 | 0.9555 | 0.3330 | 0.057* |
| C13 | 0.6453 (2) | 0.78303 (18) | 0.47387 (14) | 0.0549 (6) |
| H13A | 0.6546 | 0.7842 | 0.5412 | 0.066* |
| H13B | 0.7210 | 0.8233 | 0.4553 | 0.066* |
| C14 | 0.6128 (2) | 0.7208 (2) | 0.27315 (14) | 0.0582 (6) |
| H14A | 0.6925 | 0.7679 | 0.2787 | 0.070* |
| H14B | 0.6040 | 0.6817 | 0.2131 | 0.070* |
| C15 | 0.62998 (19) | 0.62694 (18) | 0.34763 (14) | 0.0457 (5) |
| C16 | 0.64605 (19) | 0.65618 (17) | 0.44180 (14) | 0.0444 (5) |
| C17 | 0.6686 (2) | 0.5659 (2) | 0.50689 (16) | 0.0564 (6) |
| H17 | 0.6789 | 0.5845 | 0.5699 | 0.068* |
| C18 | 0.6759 (2) | 0.4489 (2) | 0.48021 (19) | 0.0656 (7) |
| H18 | 0.6920 | 0.3898 | 0.5249 | 0.079* |
| C19 | 0.6596 (2) | 0.4205 (2) | 0.3879 (2) | 0.0677 (7) |
| H19 | 0.6643 | 0.3420 | 0.3694 | 0.081* |
| C20 | 0.6363 (2) | 0.5086 (2) | 0.32287 (17) | 0.0600 (6) |
| H20 | 0.6243 | 0.4885 | 0.2602 | 0.072* |
| N1 | 0.33311 (17) | 0.93432 (14) | 0.42804 (11) | 0.0477 (4) |
| N2 | 0.29307 (17) | 0.84723 (15) | 0.27388 (11) | 0.0487 (4) |
| N3 | 0.52758 (17) | 0.84800 (14) | 0.43754 (11) | 0.0489 (5) |
| N4 | 0.50216 (17) | 0.80036 (15) | 0.27382 (11) | 0.0493 (4) |
| O1 | 0.42173 (16) | 0.84965 (13) | 0.56762 (10) | 0.0608 (4) |
| O2 | 0.34199 (15) | 0.67820 (14) | 0.19698 (10) | 0.0660 (5) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0418 (12) | 0.0504 (13) | 0.0468 (12) | 0.0045 (10) | −0.0002 (9) | −0.0011 (10) |
| C2 | 0.0425 (13) | 0.0628 (15) | 0.0758 (17) | −0.0016 (11) | 0.0035 (12) | −0.0180 (13) |
| C3 | 0.0443 (15) | 0.0651 (17) | 0.120 (2) | −0.0110 (13) | 0.0065 (15) | 0.0016 (17) |
| C4 | 0.0596 (17) | 0.093 (2) | 0.084 (2) | −0.0135 (15) | 0.0100 (14) | 0.0250 (16) |
| C5 | 0.0598 (16) | 0.0816 (19) | 0.0520 (14) | −0.0043 (14) | 0.0078 (12) | 0.0053 (12) |
| C6 | 0.0488 (13) | 0.0438 (12) | 0.0464 (12) | 0.0040 (10) | 0.0055 (10) | 0.0007 (10) |
| C7 | 0.0733 (17) | 0.0474 (13) | 0.0477 (13) | 0.0014 (11) | 0.0107 (11) | −0.0061 (10) |
| C8 | 0.0573 (15) | 0.0741 (16) | 0.0379 (12) | 0.0006 (12) | −0.0040 (10) | −0.0028 (11) |
| C9 | 0.0732 (15) | 0.0272 (10) | 0.0391 (12) | −0.0098 (10) | 0.0025 (11) | −0.0047 (9) |
| C10 | 0.0588 (15) | 0.0515 (13) | 0.0296 (10) | −0.0040 (11) | 0.0006 (10) | 0.0026 (10) |
| C11 | 0.0641 (15) | 0.0334 (11) | 0.0424 (12) | −0.0049 (10) | 0.0062 (10) | 0.0054 (9) |
| C12 | 0.0599 (14) | 0.0391 (11) | 0.0425 (12) | −0.0105 (10) | 0.0030 (10) | 0.0020 (9) |
| C13 | 0.0672 (15) | 0.0483 (13) | 0.0447 (12) | −0.0040 (11) | −0.0082 (11) | −0.0066 (10) |
| C14 | 0.0581 (15) | 0.0751 (16) | 0.0413 (12) | 0.0033 (13) | 0.0067 (10) | −0.0051 (11) |
| C15 | 0.0386 (12) | 0.0485 (13) | 0.0493 (13) | −0.0022 (10) | 0.0037 (9) | −0.0076 (10) |
| C16 | 0.0412 (12) | 0.0414 (12) | 0.0499 (12) | −0.0027 (9) | 0.0039 (9) | −0.0027 (10) |
| C17 | 0.0536 (14) | 0.0557 (14) | 0.0611 (15) | 0.0025 (11) | 0.0125 (11) | 0.0040 (12) |
| C18 | 0.0592 (16) | 0.0475 (14) | 0.092 (2) | 0.0033 (12) | 0.0186 (14) | 0.0134 (13) |
| C19 | 0.0563 (16) | 0.0437 (14) | 0.103 (2) | −0.0019 (12) | 0.0104 (14) | −0.0104 (15) |
| C20 | 0.0451 (14) | 0.0637 (16) | 0.0699 (16) | −0.0027 (12) | 0.0037 (11) | −0.0220 (13) |
| N1 | 0.0604 (12) | 0.0393 (10) | 0.0429 (10) | −0.0058 (8) | 0.0053 (9) | −0.0045 (8) |
| N2 | 0.0516 (11) | 0.0542 (11) | 0.0386 (9) | −0.0002 (9) | 0.0004 (8) | −0.0049 (8) |
| N3 | 0.0657 (12) | 0.0402 (10) | 0.0382 (10) | 0.0041 (9) | −0.0019 (9) | −0.0024 (8) |
| N4 | 0.0541 (11) | 0.0527 (11) | 0.0409 (10) | −0.0018 (9) | 0.0054 (8) | −0.0043 (8) |
| O1 | 0.0920 (12) | 0.0513 (9) | 0.0380 (8) | −0.0111 (8) | 0.0048 (7) | −0.0027 (7) |
| O2 | 0.0781 (11) | 0.0682 (11) | 0.0487 (9) | −0.0066 (9) | −0.0016 (8) | −0.0227 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.383 (3) | C11—N2 | 1.451 (2) |
| C1—C6 | 1.397 (3) | C11—C12 | 1.536 (3) |
| C1—C8 | 1.509 (3) | C11—H11 | 0.9800 |
| C2—C3 | 1.387 (3) | C12—N4 | 1.441 (2) |
| C2—H2 | 0.9300 | C12—N3 | 1.445 (2) |
| C3—C4 | 1.365 (4) | C12—H12 | 0.9800 |
| C3—H3 | 0.9300 | C13—N3 | 1.450 (3) |
| C4—C5 | 1.369 (4) | C13—C16 | 1.507 (3) |
| C4—H4 | 0.9300 | C13—H13A | 0.9700 |
| C5—C6 | 1.380 (3) | C13—H13B | 0.9700 |
| C5—H5 | 0.9300 | C14—N4 | 1.450 (3) |
| C6—C7 | 1.506 (3) | C14—C15 | 1.508 (3) |
| C7—N1 | 1.457 (3) | C14—H14A | 0.9700 |
| C7—H7A | 0.9700 | C14—H14B | 0.9700 |
| C7—H7B | 0.9700 | C15—C20 | 1.388 (3) |
| C8—N2 | 1.444 (3) | C15—C16 | 1.394 (3) |

| | | | |
|---|---|---|---|
| C8—H8A | 0.9700 | C16—C17 | 1.388 (3) |
| C8—H8B | 0.9700 | C17—C18 | 1.382 (3) |
| C9—O1 | 1.220 (2) | C17—H17 | 0.9300 |
| C9—N3 | 1.362 (3) | C18—C19 | 1.366 (3) |
| C9—N1 | 1.374 (3) | C18—H18 | 0.9300 |
| C10—O2 | 1.223 (2) | C19—C20 | 1.371 (3) |
| C10—N2 | 1.355 (3) | C19—H19 | 0.9300 |
| C10—N4 | 1.378 (3) | C20—H20 | 0.9300 |
| C11—N1 | 1.441 (2) | | |
| C2—C1—C6 | 119.1 (2) | N4—C12—H12 | 112.0 |
| C2—C1—C8 | 119.9 (2) | N3—C12—H12 | 112.0 |
| C6—C1—C8 | 120.99 (19) | C11—C12—H12 | 112.0 |
| C1—C2—C3 | 121.1 (2) | N3—C13—C16 | 114.12 (16) |
| C1—C2—H2 | 119.5 | N3—C13—H13A | 108.7 |
| C3—C2—H2 | 119.5 | C16—C13—H13A | 108.7 |
| C4—C3—C2 | 119.4 (2) | N3—C13—H13B | 108.7 |
| C4—C3—H3 | 120.3 | C16—C13—H13B | 108.7 |
| C2—C3—H3 | 120.3 | H13A—C13—H13B | 107.6 |
| C3—C4—C5 | 120.1 (3) | N4—C14—C15 | 116.47 (17) |
| C3—C4—H4 | 120.0 | N4—C14—H14A | 108.2 |
| C5—C4—H4 | 120.0 | C15—C14—H14A | 108.2 |
| C4—C5—C6 | 121.7 (2) | N4—C14—H14B | 108.2 |
| C4—C5—H5 | 119.1 | C15—C14—H14B | 108.2 |
| C6—C5—H5 | 119.1 | H14A—C14—H14B | 107.3 |
| C5—C6—C1 | 118.6 (2) | C20—C15—C16 | 118.60 (19) |
| C5—C6—C7 | 119.6 (2) | C20—C15—C14 | 119.77 (19) |
| C1—C6—C7 | 121.82 (19) | C16—C15—C14 | 121.56 (18) |
| N1—C7—C6 | 113.92 (17) | C17—C16—C15 | 118.66 (19) |
| N1—C7—H7A | 108.8 | C17—C16—C13 | 119.73 (19) |
| C6—C7—H7A | 108.8 | C15—C16—C13 | 121.55 (18) |
| N1—C7—H7B | 108.8 | C18—C17—C16 | 121.5 (2) |
| C6—C7—H7B | 108.8 | C18—C17—H17 | 119.3 |
| H7A—C7—H7B | 107.7 | C16—C17—H17 | 119.3 |
| N2—C8—C1 | 113.52 (16) | C19—C18—C17 | 119.7 (2) |
| N2—C8—H8A | 108.9 | C19—C18—H18 | 120.1 |
| C1—C8—H8A | 108.9 | C17—C18—H18 | 120.1 |
| N2—C8—H8B | 108.9 | C18—C19—C20 | 119.4 (2) |
| C1—C8—H8B | 108.9 | C18—C19—H19 | 120.3 |
| H8A—C8—H8B | 107.7 | C20—C19—H19 | 120.3 |
| O1—C9—N3 | 126.4 (2) | C19—C20—C15 | 122.1 (2) |
| O1—C9—N1 | 125.9 (2) | C19—C20—H20 | 119.0 |
| N3—C9—N1 | 107.65 (17) | C15—C20—H20 | 119.0 |
| O2—C10—N2 | 126.4 (2) | C9—N1—C11 | 111.65 (17) |
| O2—C10—N4 | 125.5 (2) | C9—N1—C7 | 122.01 (18) |
| N2—C10—N4 | 107.99 (18) | C11—N1—C7 | 121.00 (17) |
| N1—C11—N2 | 114.20 (16) | C10—N2—C8 | 125.16 (18) |
| N1—C11—C12 | 103.60 (16) | C10—N2—C11 | 112.71 (17) |
| N2—C11—C12 | 102.33 (16) | C8—N2—C11 | 121.65 (17) |
| N1—C11—H11 | 112.0 | C9—N3—C12 | 112.86 (17) |

| | | | |
|---|---|---|---|
| N2—C11—H11 | 112.0 | C9—N3—C13 | 124.92 (17) |
| C12—C11—H11 | 112.0 | C12—N3—C13 | 122.21 (17) |
| N4—C12—N3 | 113.71 (16) | C10—N4—C12 | 110.57 (17) |
| N4—C12—C11 | 103.96 (16) | C10—N4—C14 | 122.12 (18) |
| N3—C12—C11 | 102.62 (16) | C12—N4—C14 | 120.47 (16) |
| C6—C1—C2—C3 | −0.7 (3) | N3—C9—N1—C7 | 162.83 (16) |
| C8—C1—C2—C3 | 178.5 (2) | N2—C11—N1—C9 | 97.8 (2) |
| C1—C2—C3—C4 | 1.2 (4) | C12—C11—N1—C9 | −12.7 (2) |
| C2—C3—C4—C5 | −0.3 (4) | N2—C11—N1—C7 | −56.9 (2) |
| C3—C4—C5—C6 | −1.2 (4) | C12—C11—N1—C7 | −167.34 (16) |
| C4—C5—C6—C1 | 1.7 (3) | C6—C7—N1—C9 | −76.3 (2) |
| C4—C5—C6—C7 | −178.3 (2) | C6—C7—N1—C11 | 75.7 (2) |
| C2—C1—C6—C5 | −0.8 (3) | O2—C10—N2—C8 | 4.5 (3) |
| C8—C1—C6—C5 | −179.91 (19) | N4—C10—N2—C8 | −178.65 (17) |
| C2—C1—C6—C7 | 179.28 (19) | O2—C10—N2—C11 | 176.66 (19) |
| C8—C1—C6—C7 | 0.1 (3) | N4—C10—N2—C11 | −6.5 (2) |
| C5—C6—C7—N1 | 120.4 (2) | C1—C8—N2—C10 | 94.7 (2) |
| C1—C6—C7—N1 | −59.6 (3) | C1—C8—N2—C11 | −76.8 (2) |
| C2—C1—C8—N2 | −119.7 (2) | N1—C11—N2—C10 | −114.59 (19) |
| C6—C1—C8—N2 | 59.5 (3) | C12—C11—N2—C10 | −3.4 (2) |
| N1—C11—C12—N4 | 130.26 (15) | N1—C11—N2—C8 | 57.9 (2) |
| N2—C11—C12—N4 | 11.27 (19) | C12—C11—N2—C8 | 169.12 (17) |
| N1—C11—C12—N3 | 11.55 (18) | O1—C9—N3—C12 | −177.63 (18) |
| N2—C11—C12—N3 | −107.43 (16) | N1—C9—N3—C12 | −0.1 (2) |
| N4—C14—C15—C20 | 124.7 (2) | O1—C9—N3—C13 | 3.2 (3) |
| N4—C14—C15—C16 | −58.4 (3) | N1—C9—N3—C13 | −179.29 (16) |
| C20—C15—C16—C17 | 0.4 (3) | N4—C12—N3—C9 | −119.08 (19) |
| C14—C15—C16—C17 | −176.54 (19) | C11—C12—N3—C9 | −7.5 (2) |
| C20—C15—C16—C13 | 177.8 (2) | N4—C12—N3—C13 | 60.2 (2) |
| C14—C15—C16—C13 | 0.8 (3) | C11—C12—N3—C13 | 171.78 (16) |
| N3—C13—C16—C17 | −126.3 (2) | C16—C13—N3—C9 | 102.5 (2) |
| N3—C13—C16—C15 | 56.4 (3) | C16—C13—N3—C12 | −76.7 (2) |
| C15—C16—C17—C18 | 0.4 (3) | O2—C10—N4—C12 | −168.60 (19) |
| C13—C16—C17—C18 | −177.0 (2) | N2—C10—N4—C12 | 14.5 (2) |
| C16—C17—C18—C19 | −0.6 (3) | O2—C10—N4—C14 | −17.6 (3) |
| C17—C18—C19—C20 | 0.1 (3) | N2—C10—N4—C14 | 165.55 (17) |
| C18—C19—C20—C15 | 0.7 (3) | N3—C12—N4—C10 | 94.7 (2) |
| C16—C15—C20—C19 | −1.0 (3) | C11—C12—N4—C10 | −16.1 (2) |
| C14—C15—C20—C19 | 176.1 (2) | N3—C12—N4—C14 | −56.9 (2) |
| O1—C9—N1—C11 | −173.95 (18) | C11—C12—N4—C14 | −167.67 (17) |
| N3—C9—N1—C11 | 8.5 (2) | C15—C14—N4—C10 | −74.2 (2) |
| O1—C9—N1—C7 | −19.6 (3) | C15—C14—N4—C12 | 74.1 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C19—H19···O1$^{i}$ | 0.93 | 2.55 | 3.252 (3) | 132 |
| C13—H13A···O1 | 0.97 | 2.58 | 2.924 (3) | 101 |

| | | | | |
|---|---|---|---|---|
| C7—H7A···O2$^{ii}$ | 0.97 | 2.45 | 3.343 (3) | 153 |

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

**Fig. 1**