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2,6-Diethyl-8b,8c-diphenylperhydro-2,3a,4a,6,7a,8a-hexaazacyclopenta-[*def*]fluorene-4,8-dione

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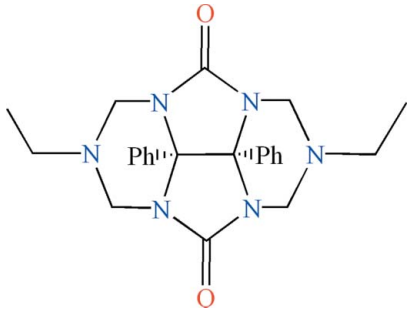
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.060; wR factor = 0.164; data-to-parameter ratio = 14.6.

The title compound, $C_{24}H_{28}N_6O_2$, is a derivative of glycoluril with two phenyl substituents on the convex face of the glycouril system. Each N atom of the separate rings of the flexible U-shaped glycoluril clip carries an ethyl substituent. Intermolecular non-classical C—H···O hydrogen bonds contribute to the stability of the crystal structure.

Related literature

For the preparation of the title compound, see: Li *et al.* (2006). For related literature, see: Degen *et al.*, (2007); Elemans *et al.* (2000); Freeman *et al.* (1981); Klarner & Kahlert (2003); Rebek (2005); Rowan *et al.* (1999); Wu *et al.* (2002).



Experimental

Crystal data

$C_{24}H_{28}N_6O_2$
M_r = 432.52
Triclinic, $P\overline{1}$
a = 8.6963 (9) Å
b = 10.3704 (10) Å
c = 13.0294 (13) Å
α = 76.885 (2)°
β = 73.233 (1)°
γ = 84.576 (1)°
V = 1095.21 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
7080 measured reflections
4255 independent reflections
2885 reflections with $I > 2\sigma(I)$
R_{int} = 0.105

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.164
S = 0.99
4255 reflections
291 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1^{i}	0.93	2.56	3.427 (3)	155
C13—H13···O2^{ii}	0.93	2.56	3.410 (3)	152
C20—H20···O2^{ii}	0.93	2.52	3.387 (3)	155

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

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: LW2043).

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supplementary materials

Acta Cryst. (2007). E**63**, o4777 [**doi:10.1107/S1600536807058400**]

2,6-Diethyl-8b,8c-diphenylperhydro-2,3a,4a,6,7a,8a-hexaazacyclopenta[*def*]fluorene-4,8-dione

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Comment

Molecular clips and tweezers are interesting because of their supramolecular properties, like self-assembling and molecular recognition of small electron-deficient guest molecules (Degen *et al.*, 2007; Klarner *et al.*, 2003). Glycoluril and its derivatives have during the past two decades established an impressive career as a building block during supramolecular chemistry (Freeman *et al.*, 1981; Rowan *et al.*, 1999; Rebek, 2005; Wu, Fettinger *et al.*, 2002). Based on glycouril, molecular clips, molecular tweezers, cucurbituril cotaxanes, molecular mapsules and molecular basket have been designed and synthesized(Rowan *et al.*, 1999; Elemans *et al.*,2000). As a part of our ongoing investigation of glycoluril derivatives (Li *et al.*, 2006), we report here the structure of the title compound (I) (Fig. 1).

The molecular structure of (I) is shown in Fig. 1. It is a flexible glycouril clip, each N atom from separate rings of which carries an ethyl substituent. Intermolecular non-classical C—H···O hydrogen bonds contribute to the stability of the structure (Table 1).

Experimental

The title compound was synthesized according to the procedure of Li, *et al.* (2006) in 12% isolated yield. Crystals of (I) suitable for X-ray data collection were obtained by slow evaporation of a chloroform and methanol solution in ratio of 15:1 at 293 K.

Refinement

All H atoms were positioned geometrically (C—H = 0.96–0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) (1.5U_{eq}(C) for methyl of the parent atoms.

Figures

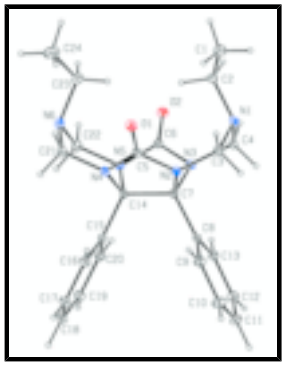


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 10% probability level. H atoms are represented by spheres of arbitrary radius.

2,6-Diethyl-8 b,8c-diphenylperhydro-2,3a,4a,6,7a,8a- hexaazacyclopenta[def]fluorene-4,8-dione

Crystal data

$C_{24}H_{28}N_6O_2$	$Z = 2$
$M_r = 432.52$	$F_{000} = 460$
Triclinic, $P\overline{1}$	$D_x = 1.312$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.6963$ (9) Å	Cell parameters from 1908 reflections
$b = 10.3704$ (10) Å	$\theta = 2.3$–23.7º
$c = 13.0294$ (13) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 76.885$ (2)º	$T = 295$ (2) K
$\beta = 73.233$ (1)º	Block, blue
$\gamma = 84.576$ (1)º	0.20 × 0.20 × 0.10 mm
$V = 1095.21$ (19) Å^3	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2885 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.105$
Monochromator: graphite	$\theta_{max} = 26.0$º
$T = 295$(2) K	$\theta_{min} = 1.7$º
φ and ω scans	$h = -10\rightarrow10$
Absorption correction: none	$k = -12\rightarrow11$
7080 measured reflections	$l = -16\rightarrow16$
4255 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
$R[F^2 > 2\sigma(F^2)] = 0.061$	H-atom parameters constrained
$wR(F^2) = 0.164$	$w = 1/[\sigma^2(F_o^2) + (0.068P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
4255 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
291 parameters	$\Delta\rho_{min} = -0.23$ 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	0.0890 (4)	−0.2902 (3)	0.9644 (2)	0.0645 (8)
H1A	0.1391	−0.2709	1.0157	0.097*
H1B	0.0987	−0.3835	0.9661	0.097*
H1C	−0.0226	−0.2635	0.9839	0.097*
C2	0.1698 (3)	−0.2160 (2)	0.8515 (2)	0.0457 (6)
H2A	0.2850	−0.2313	0.8377	0.055*
H2B	0.1362	−0.2511	0.7986	0.055*
C3	0.1908 (3)	−0.0040 (2)	0.90159 (19)	0.0391 (6)
H3A	0.1646	−0.0551	0.9763	0.047*
H3B	0.1337	0.0809	0.9023	0.047*
C4	0.1900 (3)	−0.0064 (2)	0.71965 (19)	0.0393 (6)
H4A	0.1325	0.0783	0.7091	0.047*
H4B	0.1638	−0.0592	0.6748	0.047*
C5	0.4739 (3)	−0.0717 (2)	0.89922 (18)	0.0328 (5)
C6	0.4730 (3)	−0.0729 (2)	0.63566 (17)	0.0305 (5)
C7	0.4254 (2)	0.0817 (2)	0.74911 (16)	0.0283 (5)
C8	0.3877 (2)	0.2307 (2)	0.72892 (17)	0.0299 (5)
C9	0.3722 (3)	0.2996 (2)	0.8109 (2)	0.0437 (6)
H9	0.3805	0.2550	0.8797	0.052*
C10	0.3441 (4)	0.4357 (3)	0.7899 (2)	0.0599 (8)
H10	0.3345	0.4822	0.8447	0.072*
C11	0.3304 (3)	0.5026 (3)	0.6891 (3)	0.0574 (8)
H11	0.3105	0.5937	0.6760	0.069*
C12	0.3462 (3)	0.4342 (3)	0.6077 (2)	0.0492 (7)
H12	0.3373	0.4794	0.5392	0.059*
C13	0.3753 (3)	0.2983 (2)	0.62682 (19)	0.0385 (6)
H13	0.3866	0.2526	0.5712	0.046*
C14	0.6075 (2)	0.0377 (2)	0.72159 (16)	0.0279 (5)
C15	0.7302 (2)	0.1463 (2)	0.67807 (18)	0.0314 (5)
C16	0.7865 (3)	0.1967 (2)	0.7500 (2)	0.0418 (6)
H16	0.7484	0.1649	0.8252	0.050*
C17	0.8994 (3)	0.2942 (3)	0.7098 (2)	0.0519 (7)
H17	0.9373	0.3277	0.7580	0.062*

C18	0.9557 (3)	0.3416 (3)	0.5991 (2)	0.0536 (7)
H18	1.0326	0.4064	0.5724	0.064*
C19	0.8986 (3)	0.2936 (3)	0.5272 (2)	0.0495 (7)
H19	0.9360	0.3267	0.4521	0.059*
C20	0.7859 (3)	0.1962 (2)	0.56666 (19)	0.0404 (6)
H20	0.7472	0.1641	0.5181	0.048*
C21	0.7575 (3)	−0.1426 (3)	0.8167 (2)	0.0436 (6)
H21A	0.8566	−0.0956	0.7969	0.052*
H21B	0.7471	−0.2001	0.8882	0.052*
C22	0.7572 (3)	−0.1410 (2)	0.6332 (2)	0.0455 (6)
H22A	0.7485	−0.1976	0.5853	0.055*
H22B	0.8559	−0.0931	0.5989	0.055*
C23	0.6583 (4)	−0.3353 (3)	0.7767 (2)	0.0571 (7)
H23A	0.6630	−0.3773	0.7165	0.068*
H23B	0.5492	−0.3016	0.8023	0.068*
C24	0.6991 (5)	−0.4366 (3)	0.8681 (3)	0.0896 (12)
H24A	0.8115	−0.4602	0.8471	0.134*
H24B	0.6372	−0.5139	0.8828	0.134*
H24C	0.6745	−0.4003	0.9327	0.134*
N1	0.1345 (2)	−0.07304 (19)	0.83424 (16)	0.0393 (5)
N2	0.3631 (2)	0.01826 (17)	0.86419 (14)	0.0304 (4)
N3	0.3625 (2)	0.01628 (17)	0.68186 (14)	0.0303 (4)
N4	0.6222 (2)	−0.04582 (18)	0.82483 (14)	0.0316 (4)
N5	0.6212 (2)	−0.04532 (18)	0.64235 (14)	0.0323 (4)
N6	0.7685 (2)	−0.2239 (2)	0.73700 (17)	0.0449 (5)
O1	0.4475 (2)	−0.15622 (16)	0.98420 (12)	0.0451 (5)
O2	0.4458 (2)	−0.15742 (16)	0.59266 (12)	0.0425 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.061 (2)	0.0429 (16)	0.078 (2)	−0.0049 (14)	−0.0077 (16)	−0.0041 (15)
C2	0.0360 (14)	0.0336 (14)	0.0638 (17)	−0.0038 (11)	−0.0060 (12)	−0.0119 (12)
C3	0.0284 (13)	0.0375 (13)	0.0457 (14)	−0.0013 (10)	0.0016 (10)	−0.0125 (11)
C4	0.0277 (13)	0.0391 (14)	0.0544 (15)	−0.0013 (11)	−0.0134 (11)	−0.0134 (12)
C5	0.0341 (13)	0.0350 (13)	0.0306 (12)	−0.0086 (10)	−0.0067 (10)	−0.0092 (10)
C6	0.0332 (13)	0.0301 (12)	0.0289 (12)	−0.0025 (10)	−0.0069 (10)	−0.0090 (10)
C7	0.0263 (11)	0.0292 (12)	0.0288 (11)	−0.0020 (9)	−0.0036 (9)	−0.0097 (9)
C8	0.0221 (11)	0.0277 (12)	0.0385 (13)	−0.0017 (9)	−0.0044 (9)	−0.0087 (10)
C9	0.0537 (16)	0.0340 (13)	0.0438 (14)	−0.0018 (12)	−0.0093 (12)	−0.0142 (11)
C10	0.082 (2)	0.0369 (15)	0.0650 (19)	0.0007 (15)	−0.0156 (17)	−0.0256 (14)
C11	0.0582 (19)	0.0290 (14)	0.082 (2)	0.0036 (13)	−0.0156 (16)	−0.0132 (15)
C12	0.0477 (16)	0.0362 (14)	0.0576 (17)	−0.0016 (12)	−0.0143 (13)	0.0022 (12)
C13	0.0370 (14)	0.0333 (13)	0.0438 (14)	−0.0005 (11)	−0.0081 (11)	−0.0093 (11)
C14	0.0219 (11)	0.0313 (12)	0.0301 (11)	−0.0021 (9)	−0.0039 (9)	−0.0093 (9)
C15	0.0218 (11)	0.0306 (12)	0.0393 (13)	0.0002 (9)	−0.0041 (9)	−0.0081 (10)
C16	0.0388 (14)	0.0419 (14)	0.0444 (14)	−0.0075 (11)	−0.0085 (11)	−0.0095 (11)
C17	0.0467 (16)	0.0436 (16)	0.0706 (19)	−0.0145 (13)	−0.0218 (14)	−0.0098 (14)

C18	0.0341 (15)	0.0373 (14)	0.082 (2)	−0.0126 (12)	−0.0143 (14)	0.0053 (14)
C19	0.0358 (14)	0.0463 (15)	0.0527 (16)	−0.0070 (12)	−0.0007 (12)	0.0046 (13)
C20	0.0354 (14)	0.0414 (14)	0.0401 (14)	−0.0058 (11)	−0.0043 (11)	−0.0059 (11)
C21	0.0295 (13)	0.0438 (15)	0.0566 (16)	0.0015 (11)	−0.0146 (12)	−0.0058 (12)
C22	0.0357 (14)	0.0437 (15)	0.0538 (16)	0.0073 (12)	−0.0015 (12)	−0.0214 (13)
C23	0.0547 (18)	0.0364 (15)	0.080 (2)	0.0035 (13)	−0.0194 (15)	−0.0142 (14)
C24	0.112 (3)	0.0472 (19)	0.108 (3)	−0.005 (2)	−0.039 (2)	0.0013 (19)
N1	0.0267 (10)	0.0334 (11)	0.0545 (13)	−0.0037 (9)	−0.0057 (9)	−0.0086 (9)
N2	0.0253 (10)	0.0320 (10)	0.0300 (10)	−0.0041 (8)	0.0005 (8)	−0.0078 (8)
N3	0.0256 (10)	0.0302 (10)	0.0369 (10)	−0.0012 (8)	−0.0074 (8)	−0.0118 (8)
N4	0.0255 (10)	0.0324 (10)	0.0352 (10)	−0.0023 (8)	−0.0066 (8)	−0.0051 (8)
N5	0.0282 (10)	0.0330 (10)	0.0342 (10)	0.0028 (8)	−0.0027 (8)	−0.0136 (8)
N6	0.0329 (12)	0.0394 (12)	0.0598 (14)	0.0054 (9)	−0.0105 (10)	−0.0110 (10)
O1	0.0485 (11)	0.0458 (10)	0.0347 (9)	−0.0089 (8)	−0.0067 (8)	0.0011 (8)
O2	0.0494 (11)	0.0406 (9)	0.0439 (10)	−0.0024 (8)	−0.0132 (8)	−0.0206 (8)

Geometric parameters (Å, °)

C1—C2	1.497 (3)	C12—C13	1.387 (3)
C1—H1A	0.9600	C12—H12	0.9300
C1—H1B	0.9600	C13—H13	0.9300
C1—H1C	0.9600	C14—N4	1.458 (3)
C2—N1	1.465 (3)	C14—N5	1.461 (3)
C2—H2A	0.9700	C14—C15	1.522 (3)
C2—H2B	0.9700	C15—C20	1.382 (3)
C3—N1	1.457 (3)	C15—C16	1.388 (3)
C3—N2	1.459 (3)	C16—C17	1.382 (3)
C3—H3A	0.9700	C16—H16	0.9300
C3—H3B	0.9700	C17—C18	1.370 (4)
C4—N1	1.456 (3)	C17—H17	0.9300
C4—N3	1.461 (3)	C18—C19	1.378 (4)
C4—H4A	0.9700	C18—H18	0.9300
C4—H4B	0.9700	C19—C20	1.380 (3)
C5—O1	1.224 (2)	C19—H19	0.9300
C5—N2	1.377 (3)	C20—H20	0.9300
C5—N4	1.379 (3)	C21—N6	1.458 (3)
C6—O2	1.216 (2)	C21—N4	1.468 (3)
C6—N3	1.375 (3)	C21—H21A	0.9700
C6—N5	1.377 (3)	C21—H21B	0.9700
C7—N2	1.458 (3)	C22—N6	1.453 (3)
C7—N3	1.464 (2)	C22—N5	1.466 (3)
C7—C8	1.528 (3)	C22—H22A	0.9700
C7—C14	1.566 (3)	C22—H22B	0.9700
C8—C9	1.384 (3)	C23—N6	1.474 (3)
C8—C13	1.385 (3)	C23—C24	1.500 (4)
C9—C10	1.387 (4)	C23—H23A	0.9700
C9—H9	0.9300	C23—H23B	0.9700
C10—C11	1.371 (4)	C24—H24A	0.9600
C10—H10	0.9300	C24—H24B	0.9600

C11—C12	1.373 (4)	C24—H24C	0.9600
C11—H11	0.9300		
C2—C1—H1A	109.5	C20—C15—C16	119.4 (2)
C2—C1—H1B	109.5	C20—C15—C14	120.36 (19)
H1A—C1—H1B	109.5	C16—C15—C14	120.3 (2)
C2—C1—H1C	109.5	C17—C16—C15	119.9 (2)
H1A—C1—H1C	109.5	C17—C16—H16	120.0
H1B—C1—H1C	109.5	C15—C16—H16	120.0
N1—C2—C1	113.7 (2)	C18—C17—C16	120.3 (2)
N1—C2—H2A	108.8	C18—C17—H17	119.9
C1—C2—H2A	108.8	C16—C17—H17	119.9
N1—C2—H2B	108.8	C17—C18—C19	120.2 (2)
C1—C2—H2B	108.8	C17—C18—H18	119.9
H2A—C2—H2B	107.7	C19—C18—H18	119.9
N1—C3—N2	113.90 (18)	C18—C19—C20	119.9 (2)
N1—C3—H3A	108.8	C18—C19—H19	120.0
N2—C3—H3A	108.8	C20—C19—H19	120.0
N1—C3—H3B	108.8	C19—C20—C15	120.3 (2)
N2—C3—H3B	108.8	C19—C20—H20	119.8
H3A—C3—H3B	107.7	C15—C20—H20	119.8
N1—C4—N3	113.84 (18)	N6—C21—N4	113.91 (18)
N1—C4—H4A	108.8	N6—C21—H21A	108.8
N3—C4—H4A	108.8	N4—C21—H21A	108.8
N1—C4—H4B	108.8	N6—C21—H21B	108.8
N3—C4—H4B	108.8	N4—C21—H21B	108.8
H4A—C4—H4B	107.7	H21A—C21—H21B	107.7
O1—C5—N2	126.2 (2)	N6—C22—N5	114.39 (19)
O1—C5—N4	125.5 (2)	N6—C22—H22A	108.7
N2—C5—N4	108.24 (18)	N5—C22—H22A	108.7
O2—C6—N3	126.1 (2)	N6—C22—H22B	108.7
O2—C6—N5	126.1 (2)	N5—C22—H22B	108.7
N3—C6—N5	107.80 (17)	H22A—C22—H22B	107.6
N2—C7—N3	109.20 (15)	N6—C23—C24	112.2 (2)
N2—C7—C8	111.82 (17)	N6—C23—H23A	109.2
N3—C7—C8	112.05 (17)	C24—C23—H23A	109.2
N2—C7—C14	103.45 (16)	N6—C23—H23B	109.2
N3—C7—C14	103.08 (16)	C24—C23—H23B	109.2
C8—C7—C14	116.52 (16)	H23A—C23—H23B	107.9
C9—C8—C13	119.7 (2)	C23—C24—H24A	109.5
C9—C8—C7	120.3 (2)	C23—C24—H24B	109.5
C13—C8—C7	119.94 (19)	H24A—C24—H24B	109.5
C8—C9—C10	119.5 (2)	C23—C24—H24C	109.5
C8—C9—H9	120.2	H24A—C24—H24C	109.5
C10—C9—H9	120.2	H24B—C24—H24C	109.5
C11—C10—C9	120.8 (2)	C4—N1—C3	109.47 (17)
C11—C10—H10	119.6	C4—N1—C2	112.71 (19)
C9—C10—H10	119.6	C3—N1—C2	115.28 (19)
C10—C11—C12	119.6 (2)	C5—N2—C7	111.13 (17)
C10—C11—H11	120.2	C5—N2—C3	122.64 (18)

C12—C11—H11	120.2	C7—N2—C3	115.74 (17)
C11—C12—C13	120.5 (2)	C6—N3—C4	122.70 (18)
C11—C12—H12	119.8	C6—N3—C7	111.66 (17)
C13—C12—H12	119.8	C4—N3—C7	115.74 (17)
C8—C13—C12	119.8 (2)	C5—N4—C14	111.48 (18)
C8—C13—H13	120.1	C5—N4—C21	123.05 (19)
C12—C13—H13	120.1	C14—N4—C21	115.96 (18)
N4—C14—N5	109.15 (17)	C6—N5—C14	111.84 (17)
N4—C14—C15	111.90 (16)	C6—N5—C22	123.01 (19)
N5—C14—C15	111.68 (17)	C14—N5—C22	115.18 (17)
N4—C14—C7	102.98 (15)	C22—N6—C21	110.28 (18)
N5—C14—C7	102.89 (15)	C22—N6—C23	113.4 (2)
C15—C14—C7	117.46 (18)	C21—N6—C23	114.3 (2)
N2—C7—C8—C9	29.1 (3)	C14—C7—N2—C5	−10.5 (2)
N3—C7—C8—C9	152.1 (2)	N3—C7—N2—C3	−47.2 (2)
C14—C7—C8—C9	−89.6 (2)	C8—C7—N2—C3	77.4 (2)
N2—C7—C8—C13	−153.51 (19)	C14—C7—N2—C3	−156.44 (17)
N3—C7—C8—C13	−30.5 (3)	N1—C3—N2—C5	−89.5 (2)
C14—C7—C8—C13	87.8 (2)	N1—C3—N2—C7	52.2 (3)
C13—C8—C9—C10	0.1 (4)	O2—C6—N3—C4	22.0 (3)
C7—C8—C9—C10	177.5 (2)	N5—C6—N3—C4	−160.69 (18)
C8—C9—C10—C11	0.5 (4)	O2—C6—N3—C7	166.1 (2)
C9—C10—C11—C12	−0.6 (4)	N5—C6—N3—C7	−16.6 (2)
C10—C11—C12—C13	0.2 (4)	N1—C4—N3—C6	91.0 (2)
C9—C8—C13—C12	−0.5 (3)	N1—C4—N3—C7	−51.7 (3)
C7—C8—C13—C12	−177.9 (2)	N2—C7—N3—C6	−99.8 (2)
C11—C12—C13—C8	0.4 (4)	C8—C7—N3—C6	135.78 (19)
N2—C7—C14—N4	0.65 (18)	C14—C7—N3—C6	9.7 (2)
N3—C7—C14—N4	−113.10 (16)	N2—C7—N3—C4	47.0 (2)
C8—C7—C14—N4	123.77 (18)	C8—C7—N3—C4	−77.4 (2)
N2—C7—C14—N5	114.10 (16)	C14—C7—N3—C4	156.51 (17)
N3—C7—C14—N5	0.36 (19)	O1—C5—N4—C14	166.56 (19)
C8—C7—C14—N5	−122.78 (18)	N2—C5—N4—C14	−16.5 (2)
N2—C7—C14—C15	−122.80 (18)	O1—C5—N4—C21	21.7 (3)
N3—C7—C14—C15	123.45 (18)	N2—C5—N4—C21	−161.32 (18)
C8—C7—C14—C15	0.3 (3)	N5—C14—N4—C5	−99.4 (2)
N4—C14—C15—C20	151.3 (2)	C15—C14—N4—C5	136.47 (19)
N5—C14—C15—C20	28.6 (3)	C7—C14—N4—C5	9.4 (2)
C7—C14—C15—C20	−89.9 (3)	N5—C14—N4—C21	48.1 (2)
N4—C14—C15—C16	−29.1 (3)	C15—C14—N4—C21	−76.0 (2)
N5—C14—C15—C16	−151.8 (2)	C7—C14—N4—C21	156.92 (17)
C7—C14—C15—C16	89.7 (2)	N6—C21—N4—C5	92.6 (3)
C20—C15—C16—C17	−1.1 (4)	N6—C21—N4—C14	−50.8 (3)
C14—C15—C16—C17	179.2 (2)	O2—C6—N5—C14	−165.8 (2)
C15—C16—C17—C18	0.1 (4)	N3—C6—N5—C14	16.9 (2)
C16—C17—C18—C19	0.8 (4)	O2—C6—N5—C22	−22.0 (3)
C17—C18—C19—C20	−0.8 (4)	N3—C6—N5—C22	160.70 (19)
C18—C19—C20—C15	−0.2 (4)	N4—C14—N5—C6	98.52 (19)
C16—C15—C20—C19	1.1 (4)	C15—C14—N5—C6	−137.22 (19)

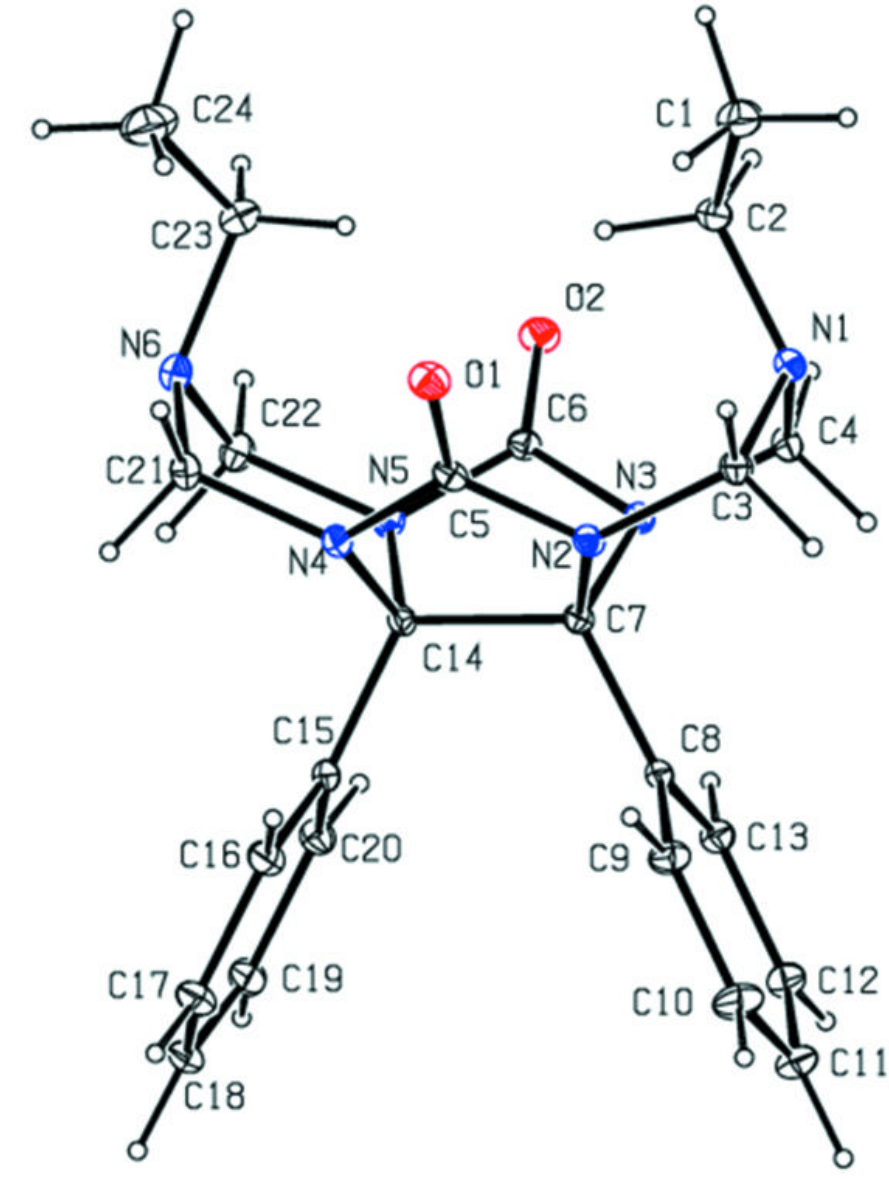
C14—C15—C20—C19	−179.2 (2)	C7—C14—N5—C6	−10.3 (2)
N3—C4—N1—C3	51.3 (2)	N4—C14—N5—C22	−48.3 (2)
N3—C4—N1—C2	−78.4 (2)	C15—C14—N5—C22	76.0 (2)
N2—C3—N1—C4	−51.5 (2)	C7—C14—N5—C22	−157.17 (17)
N2—C3—N1—C2	76.7 (3)	N6—C22—N5—C6	−90.8 (2)
C1—C2—N1—C4	−169.8 (2)	N6—C22—N5—C14	51.9 (3)
C1—C2—N1—C3	63.6 (3)	N5—C22—N6—C21	−49.9 (3)
O1—C5—N2—C7	−166.2 (2)	N5—C22—N6—C23	79.8 (3)
N4—C5—N2—C7	16.9 (2)	N4—C21—N6—C22	49.0 (3)
O1—C5—N2—C3	−23.0 (3)	N4—C21—N6—C23	−80.2 (3)
N4—C5—N2—C3	160.07 (18)	C24—C23—N6—C22	166.3 (3)
N3—C7—N2—C5	98.73 (19)	C24—C23—N6—C21	−66.1 (3)
C8—C7—N2—C5	−136.70 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O1^{i}	0.93	2.56	3.427 (3)	155
C13—H13···O2^{ii}	0.93	2.56	3.410 (3)	152
C20—H20···O2^{ii}	0.93	2.52	3.387 (3)	155

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

Fig. 1


C24
C1
C23
C2
O2
N6
N1
O1
C6
C22
C4
C21
N5
N3
C3
C5
N4
N2
C7
C14
C15
C8
C16
C20
C9
C13
C17
C19
C10
C12
C18
C11