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2,2′-Diethyl-1,1′-(4-oxoheptane-1,7-diyl)di-1*H*-benzimidazole

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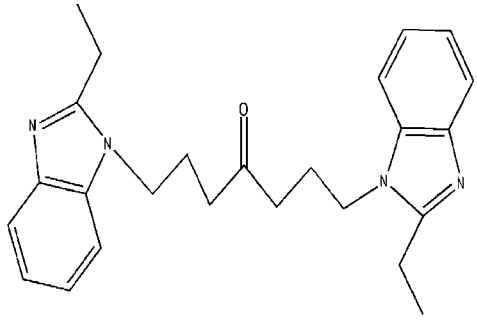
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.130; data-to-parameter ratio = 19.5.

The title compound, $C_{25}H_{30}N_4O$, was synthesized by acidic hydrolysis of its ketal precursor. The benzimidazole ring systems form a dihedral angle of 86.66 (3)°. The crystal packing is governed only by van der Waals interactions. The molecular conformation is influenced by an intramolecular C—H···N hydrogen bond.

Related literature

For related literature, see: Ma *et al.* (2004).



Experimental

Crystal data

$C_{25}H_{30}N_4O$
M_r = 402.53
Monoclinic, $P2_1/c$
a = 10.886 (7) Å
b = 9.526 (6) Å
c = 21.734 (14) Å
β = 102.672 (12)°
V = 2199 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.982
13412 measured reflections
5291 independent reflections
2889 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.130
S = 1.01
5291 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···N1	0.97	2.61	2.999 (2)	105

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2173).

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supplementary materials

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2,2'-Diethyl-1,1'-(4-oxoheptane-1,7-diyl)di-1*H*-benzimidazole

L.-P. Zhang, J.-F. Ma, Z.-F. Jia and G.-H. Wei

Comment

Bis(imidazole), which can be used to produce coordination polymic materials, is a divergent bidentate ligand commonly used as a flexible bridging ligand (Ma *et al.*, 2004). Hence, complexes of bis(imidazole) and its derivatives are studied widely. In this paper, the synthesis and structure of the title compound is reported.

In the title compound (Fig. 1), the benzimidazole rings are substantially planar, with maximum deviations of 0.010 (2) and 0.0092 (16) Å for atoms C5 and C23, respectively, and form a dihedral angle of 86.66 (3) °. The molecular conformation is stabilized by a weak intramolecular C—H···N hydrogen bond (Table 1). The crystal packing is governed only by van der Waals interactions.

Experimental

To a solution of 1,7-dichloro-4-oxoheptane (5.3 g, 3.0 mmol) and ethylene glycol (1.9 g, 3.0 mmol) in cyclohexane (22.5 ml) sodium bisulfate (0.015 g) was added. The reaction mixture was refluxed for 3 h with azeotropic removal of water *via* a Dean-Stark trap. The resulting clear solution was cooled down, washed with water twice, and then distilled. The distillation fraction between 447 and 453 K was collected. A mixture of 2-ethyl-benzimidazole (7.3 g, 50 mmol) and NaOH (2.0 g, 50 mmol) in DMSO (10 ml) was stirred at 333 K for 1 h, then the collected distillation fraction (5.5 g, 25 mmol) was added. The mixture was cooled to room temperature after stirring at 333 K for 2 h, then poured into of water (200 ml) to form immediately a white precipitate. After washing with water (50 ml), the solid was transferred to a solution of 12 *M* HCl in water (150 ml). The mixture was refluxed for 3.5 h, filtered off, and the residue (0.20 g) dissolved in methanol (15 ml). Colourless single crystals of the title compound were obtained after several days on slow evaporation of the solvent at room temperature.

Refinement

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

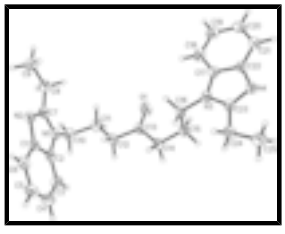


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

2,2'-Diethyl-1,1'-(4-oxoheptane-1,7-diyl)di-1*H*-benzimidazole

Crystal data

$C_{25}H_{30}N_4O$	F_{000} = 864
M_r = 402.53	D_x = 1.216 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: not measured K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71069 Å
a = 10.886 (7) Å	Cell parameters from 5291 reflections
b = 9.526 (6) Å	θ = 1.9–28.3º
c = 21.734 (14) Å	μ = 0.08 mm^{-1}
β = 102.672 (12)º	T = 293 (2) K
V = 2199 (2) Å^3	Block, colourless
Z = 4	0.40 × 0.30 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer	5291 independent reflections
Radiation source: fine-focus sealed tube	2889 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.059
T = 293(2) K	θ_{max} = 28.3º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −14→10
T_{min} = 0.970, T_{max} = 0.982	k = −8→12
13412 measured reflections	l = −27→28

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$w = 1/[\sigma^2(F_o^2) + (0.053P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.130	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.01	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
5291 reflections	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
272 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0029 (7)
Secondary atom site location: difference Fourier map	

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	0.65136 (15)	0.65380 (17)	0.54635 (8)	0.0482 (4)
C2	0.72914 (15)	0.61470 (17)	0.50605 (7)	0.0469 (4)
C3	0.77365 (18)	0.7109 (2)	0.46823 (9)	0.0638 (5)
H3	0.8260	0.6839	0.4418	0.077*
C4	0.7366 (2)	0.8478 (2)	0.47173 (10)	0.0760 (6)
H4	0.7640	0.9151	0.4468	0.091*
C5	0.6594 (2)	0.8886 (2)	0.51142 (11)	0.0737 (6)
H5	0.6361	0.9824	0.5123	0.088*
C6	0.61636 (18)	0.79397 (19)	0.54961 (9)	0.0610 (5)
H6	0.5657	0.8224	0.5766	0.073*
C7	0.67739 (15)	0.43185 (17)	0.55765 (7)	0.0452 (4)
C8	0.67221 (18)	0.28324 (18)	0.57800 (9)	0.0594 (5)
H8A	0.7570	0.2520	0.5966	0.071*
H8B	0.6408	0.2257	0.5411	0.071*
C9	0.5908 (2)	0.2596 (2)	0.62469 (10)	0.0741 (6)
H9A	0.5918	0.1618	0.6355	0.111*
H9B	0.5061	0.2881	0.6064	0.111*
H9C	0.6226	0.3138	0.6620	0.111*
C10	0.82124 (15)	0.38095 (19)	0.48254 (8)	0.0557 (5)
H10A	0.8686	0.3159	0.5131	0.067*
H10B	0.8812	0.4385	0.4669	0.067*
C11	0.74318 (17)	0.29774 (18)	0.42782 (8)	0.0559 (5)
H11A	0.7993	0.2426	0.4084	0.067*
H11B	0.6891	0.2331	0.4441	0.067*
C12	0.66271 (15)	0.38945 (17)	0.37815 (7)	0.0498 (4)
H12A	0.6143	0.4523	0.3988	0.060*
H12B	0.7179	0.4469	0.3591	0.060*
C13	0.57347 (16)	0.31317 (19)	0.32671 (8)	0.0492 (4)
C14	0.50134 (16)	0.40223 (18)	0.27465 (8)	0.0554 (5)
H14A	0.5587	0.4338	0.2491	0.066*
H14B	0.4720	0.4849	0.2932	0.066*
C15	0.38883 (15)	0.33353 (19)	0.23140 (8)	0.0536 (4)
H15A	0.3705	0.3823	0.1912	0.064*

H15B	0.4096	0.2370	0.2236	0.064*
C16	0.27321 (15)	0.33575 (17)	0.25925 (8)	0.0503 (4)
H16A	0.2922	0.2899	0.3001	0.060*
H16B	0.2504	0.4323	0.2655	0.060*
C17	0.13936 (14)	0.12333 (17)	0.21942 (7)	0.0430 (4)
C18	0.19173 (16)	0.01599 (19)	0.25986 (8)	0.0554 (5)
H18	0.2589	0.0317	0.2938	0.067*
C19	0.13911 (18)	−0.1150 (2)	0.24709 (9)	0.0628 (5)
H19	0.1716	−0.1899	0.2731	0.075*
C20	0.03894 (18)	−0.13853 (19)	0.19652 (10)	0.0615 (5)
H20	0.0061	−0.2287	0.1894	0.074*
C22	0.03816 (14)	0.10199 (17)	0.16846 (7)	0.0446 (4)
C23	0.08260 (15)	0.32118 (17)	0.16817 (7)	0.0453 (4)
C24	0.07978 (17)	0.47399 (17)	0.15393 (9)	0.0598 (5)
H25A	0.1615	0.5023	0.1472	0.072*
H25B	0.0647	0.5254	0.1901	0.072*
C25	−0.0204 (2)	0.5131 (2)	0.09637 (10)	0.0763 (6)
H28A	−0.0182	0.6125	0.0895	0.115*
H28B	−0.1017	0.4871	0.1030	0.115*
H28C	−0.0047	0.4645	0.0602	0.115*
C21	−0.01315 (17)	−0.03124 (18)	0.15657 (9)	0.0552 (5)
HC22	−0.0805	−0.0477	0.1228	0.066*
N1	0.74548 (13)	0.47145 (14)	0.51418 (6)	0.0475 (3)
N2	0.62039 (13)	0.53759 (14)	0.57860 (6)	0.0504 (4)
N3	0.16700 (12)	0.26482 (14)	0.21831 (6)	0.0453 (3)
N4	0.00414 (13)	0.22733 (13)	0.13691 (6)	0.0485 (4)
O1	0.55972 (14)	0.18762 (14)	0.32768 (6)	0.0850 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0457 (10)	0.0517 (10)	0.0449 (10)	−0.0032 (8)	0.0051 (8)	−0.0033 (8)
C2	0.0402 (9)	0.0563 (11)	0.0414 (9)	−0.0043 (8)	0.0030 (8)	−0.0018 (8)
C3	0.0585 (12)	0.0785 (14)	0.0550 (12)	−0.0125 (10)	0.0134 (10)	0.0016 (10)
C4	0.0788 (15)	0.0675 (14)	0.0791 (15)	−0.0175 (12)	0.0117 (13)	0.0124 (11)
C5	0.0772 (15)	0.0498 (11)	0.0891 (16)	−0.0091 (10)	0.0071 (13)	−0.0001 (11)
C6	0.0615 (12)	0.0549 (12)	0.0656 (12)	−0.0018 (9)	0.0119 (10)	−0.0105 (9)
C7	0.0382 (9)	0.0550 (10)	0.0406 (9)	0.0009 (8)	0.0048 (8)	−0.0015 (8)
C8	0.0560 (11)	0.0581 (11)	0.0628 (12)	0.0041 (9)	0.0101 (10)	0.0031 (9)
C9	0.0739 (14)	0.0712 (13)	0.0803 (15)	0.0056 (11)	0.0235 (12)	0.0216 (10)
C10	0.0437 (10)	0.0759 (12)	0.0457 (10)	0.0116 (9)	0.0061 (8)	−0.0069 (8)
C11	0.0525 (11)	0.0642 (11)	0.0492 (10)	0.0139 (9)	0.0074 (9)	−0.0079 (8)
C12	0.0451 (10)	0.0583 (11)	0.0448 (10)	−0.0009 (8)	0.0075 (8)	−0.0071 (8)
C13	0.0468 (10)	0.0517 (11)	0.0494 (10)	−0.0029 (8)	0.0110 (8)	−0.0094 (8)
C14	0.0429 (10)	0.0659 (12)	0.0540 (11)	−0.0085 (9)	0.0038 (9)	−0.0005 (9)
C15	0.0435 (10)	0.0700 (12)	0.0455 (10)	−0.0061 (8)	0.0059 (8)	−0.0079 (8)
C16	0.0416 (9)	0.0626 (11)	0.0442 (10)	−0.0042 (8)	0.0040 (8)	−0.0107 (8)
C17	0.0355 (9)	0.0522 (10)	0.0434 (9)	0.0027 (7)	0.0129 (7)	−0.0002 (7)

C18	0.0475 (10)	0.0676 (12)	0.0508 (11)	0.0089 (9)	0.0099 (9)	0.0052 (9)
C19	0.0628 (12)	0.0607 (12)	0.0688 (13)	0.0142 (10)	0.0228 (11)	0.0179 (10)
C20	0.0619 (12)	0.0484 (11)	0.0781 (14)	−0.0013 (9)	0.0241 (11)	0.0010 (9)
C22	0.0377 (9)	0.0504 (10)	0.0458 (9)	−0.0002 (8)	0.0096 (8)	−0.0011 (8)
C23	0.0403 (9)	0.0494 (10)	0.0455 (10)	0.0024 (8)	0.0078 (8)	−0.0015 (7)
C24	0.0578 (12)	0.0537 (11)	0.0652 (12)	−0.0004 (9)	0.0075 (10)	−0.0001 (9)
C25	0.0733 (14)	0.0630 (12)	0.0844 (15)	0.0040 (10)	−0.0006 (12)	0.0166 (10)
C21	0.0489 (10)	0.0558 (11)	0.0597 (11)	−0.0037 (9)	0.0096 (9)	−0.0045 (9)
N1	0.0425 (8)	0.0574 (9)	0.0415 (8)	0.0015 (6)	0.0068 (7)	−0.0060 (6)
N2	0.0482 (9)	0.0537 (9)	0.0505 (9)	0.0012 (7)	0.0136 (7)	−0.0025 (7)
N3	0.0356 (7)	0.0533 (9)	0.0444 (8)	−0.0004 (6)	0.0034 (6)	−0.0037 (6)
N4	0.0442 (8)	0.0489 (8)	0.0483 (8)	−0.0016 (6)	0.0012 (7)	−0.0002 (6)
O1	0.1068 (12)	0.0570 (9)	0.0758 (10)	−0.0034 (8)	−0.0132 (9)	−0.0089 (7)

Geometric parameters (Å, °)

C1—N2	1.391 (2)	C13—C14	1.492 (2)
C1—C6	1.395 (2)	C14—C15	1.519 (2)
C1—C2	1.396 (2)	C14—H14A	0.9700
C2—N1	1.382 (2)	C14—H14B	0.9700
C2—C3	1.388 (2)	C15—C16	1.512 (2)
C3—C4	1.372 (3)	C15—H15A	0.9700
C3—H3	0.9300	C15—H15B	0.9700
C4—C5	1.385 (3)	C16—N3	1.461 (2)
C4—H4	0.9300	C16—H16A	0.9700
C5—C6	1.376 (3)	C16—H16B	0.9700
C5—H5	0.9300	C17—N3	1.3823 (19)
C6—H6	0.9300	C17—C18	1.387 (2)
C7—N2	1.316 (2)	C17—C22	1.395 (2)
C7—N1	1.375 (2)	C18—C19	1.376 (2)
C7—C8	1.488 (2)	C18—H18	0.9300
C8—C9	1.503 (3)	C19—C20	1.386 (3)
C8—H8A	0.9700	C19—H19	0.9300
C8—H8B	0.9700	C20—C21	1.380 (2)
C9—H9A	0.9600	C20—H20	0.9300
C9—H9B	0.9600	C22—N4	1.386 (2)
C9—H9C	0.9600	C22—C21	1.388 (2)
C10—N1	1.465 (2)	C23—N4	1.3175 (19)
C10—C11	1.524 (2)	C23—N3	1.371 (2)
C10—H10A	0.9700	C23—C24	1.487 (2)
C10—H10B	0.9700	C24—C25	1.515 (2)
C11—C12	1.510 (2)	C24—H25A	0.9700
C11—H11A	0.9700	C24—H25B	0.9700
C11—H11B	0.9700	C25—H28A	0.9600
C12—C13	1.498 (2)	C25—H28B	0.9600
C12—H12A	0.9700	C25—H28C	0.9600
C12—H12B	0.9700	C21—HC22	0.9300
C13—O1	1.206 (2)		
N2—C1—C6	129.60 (17)	C13—C14—H14B	108.2

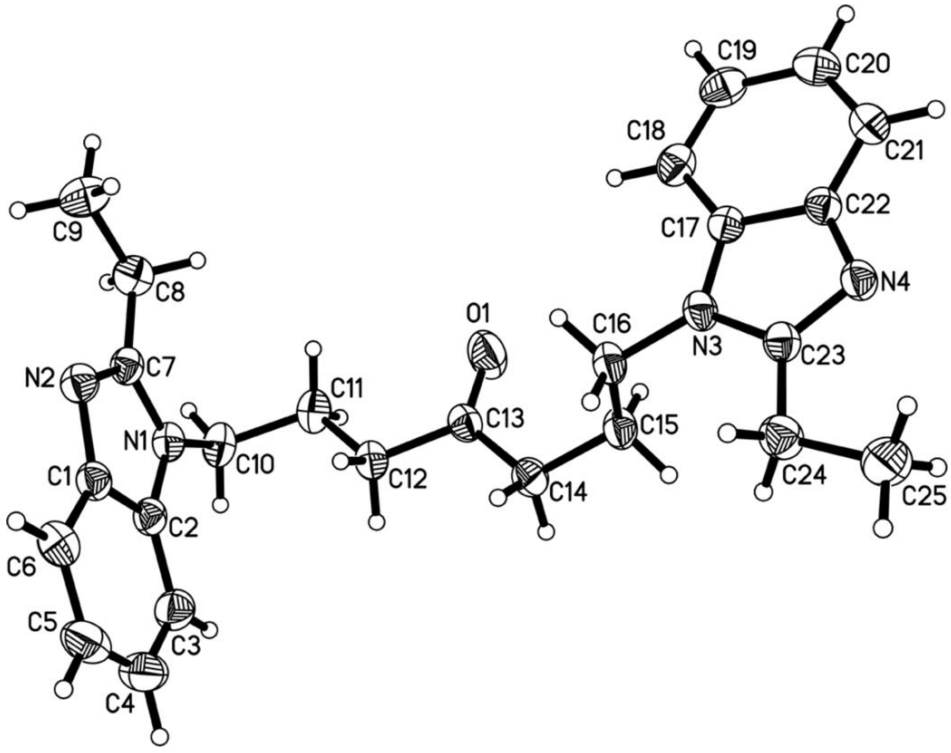
N2—C1—C2	110.57 (14)	C15—C14—H14B	108.2
C6—C1—C2	119.83 (16)	H14A—C14—H14B	107.4
N1—C2—C3	132.53 (17)	C16—C15—C14	112.05 (14)
N1—C2—C1	105.19 (14)	C16—C15—H15A	109.2
C3—C2—C1	122.29 (17)	C14—C15—H15A	109.2
C4—C3—C2	116.74 (19)	C16—C15—H15B	109.2
C4—C3—H3	121.6	C14—C15—H15B	109.2
C2—C3—H3	121.6	H15A—C15—H15B	107.9
C3—C4—C5	121.81 (19)	N3—C16—C15	111.53 (13)
C3—C4—H4	119.1	N3—C16—H16A	109.3
C5—C4—H4	119.1	C15—C16—H16A	109.3
C6—C5—C4	121.68 (19)	N3—C16—H16B	109.3
C6—C5—H5	119.2	C15—C16—H16B	109.3
C4—C5—H5	119.2	H16A—C16—H16B	108.0
C5—C6—C1	117.65 (19)	N3—C17—C18	132.01 (15)
C5—C6—H6	121.2	N3—C17—C22	105.38 (13)
C1—C6—H6	121.2	C18—C17—C22	122.61 (16)
N2—C7—N1	113.20 (15)	C19—C18—C17	116.49 (16)
N2—C7—C8	125.03 (16)	C19—C18—H18	121.8
N1—C7—C8	121.77 (15)	C17—C18—H18	121.8
C7—C8—C9	114.17 (15)	C18—C19—C20	121.77 (17)
C7—C8—H8A	108.7	C18—C19—H19	119.1
C9—C8—H8A	108.7	C20—C19—H19	119.1
C7—C8—H8B	108.7	C21—C20—C19	121.51 (17)
C9—C8—H8B	108.7	C21—C20—H20	119.2
H8A—C8—H8B	107.6	C19—C20—H20	119.2
C8—C9—H9A	109.5	N4—C22—C21	129.99 (15)
C8—C9—H9B	109.5	N4—C22—C17	110.24 (14)
H9A—C9—H9B	109.5	C21—C22—C17	119.77 (15)
C8—C9—H9C	109.5	N4—C23—N3	112.93 (14)
H9A—C9—H9C	109.5	N4—C23—C24	125.13 (14)
H9B—C9—H9C	109.5	N3—C23—C24	121.89 (14)
N1—C10—C11	113.43 (13)	C23—C24—C25	113.01 (15)
N1—C10—H10A	108.9	C23—C24—H25A	109.0
C11—C10—H10A	108.9	C25—C24—H25A	109.0
N1—C10—H10B	108.9	C23—C24—H25B	109.0
C11—C10—H10B	108.9	C25—C24—H25B	109.0
H10A—C10—H10B	107.7	H25A—C24—H25B	107.8
C12—C11—C10	113.19 (14)	C24—C25—H28A	109.5
C12—C11—H11A	108.9	C24—C25—H28B	109.5
C10—C11—H11A	108.9	H28A—C25—H28B	109.5
C12—C11—H11B	108.9	C24—C25—H28C	109.5
C10—C11—H11B	108.9	H28A—C25—H28C	109.5
H11A—C11—H11B	107.8	H28B—C25—H28C	109.5
C13—C12—C11	115.61 (14)	C20—C21—C22	117.85 (17)
C13—C12—H12A	108.4	C20—C21—HC22	121.1
C11—C12—H12A	108.4	C22—C21—HC22	121.1
C13—C12—H12B	108.4	C7—N1—C2	106.55 (13)
C11—C12—H12B	108.4	C7—N1—C10	127.23 (15)

H12A—C12—H12B	107.4	C2—N1—C10	126.22 (15)
O1—C13—C14	122.03 (15)	C7—N2—C1	104.48 (14)
O1—C13—C12	122.04 (15)	C23—N3—C17	106.57 (12)
C14—C13—C12	115.92 (15)	C23—N3—C16	127.28 (14)
C13—C14—C15	116.30 (14)	C17—N3—C16	125.91 (13)
C13—C14—H14A	108.2	C23—N4—C22	104.88 (13)
C15—C14—H14A	108.2		
N2—C1—C2—N1	0.01 (17)	C19—C20—C21—C22	0.1 (3)
C6—C1—C2—N1	179.88 (14)	N4—C22—C21—C20	−179.22 (17)
N2—C1—C2—C3	179.89 (14)	C17—C22—C21—C20	0.2 (2)
C6—C1—C2—C3	−0.2 (2)	N2—C7—N1—C2	−0.86 (17)
N1—C2—C3—C4	179.29 (17)	C8—C7—N1—C2	179.63 (14)
C1—C2—C3—C4	−0.6 (3)	N2—C7—N1—C10	178.92 (13)
C2—C3—C4—C5	0.5 (3)	C8—C7—N1—C10	−0.6 (2)
C3—C4—C5—C6	0.3 (3)	C3—C2—N1—C7	−179.39 (17)
C4—C5—C6—C1	−1.1 (3)	C1—C2—N1—C7	0.47 (16)
N2—C1—C6—C5	−179.12 (17)	C3—C2—N1—C10	0.8 (3)
C2—C1—C6—C5	1.0 (2)	C1—C2—N1—C10	−179.31 (14)
N2—C7—C8—C9	1.9 (2)	C11—C10—N1—C7	79.0 (2)
N1—C7—C8—C9	−178.70 (15)	C11—C10—N1—C2	−101.27 (19)
N1—C10—C11—C12	57.0 (2)	N1—C7—N2—C1	0.84 (17)
C10—C11—C12—C13	−173.63 (15)	C8—C7—N2—C1	−179.67 (15)
C11—C12—C13—O1	5.7 (2)	C6—C1—N2—C7	179.64 (16)
C11—C12—C13—C14	−175.12 (15)	C2—C1—N2—C7	−0.51 (17)
O1—C13—C14—C15	13.9 (3)	N4—C23—N3—C17	−0.53 (18)
C12—C13—C14—C15	−165.28 (15)	C24—C23—N3—C17	177.05 (15)
C13—C14—C15—C16	82.0 (2)	N4—C23—N3—C16	174.15 (14)
C14—C15—C16—N3	−177.89 (13)	C24—C23—N3—C16	−8.3 (2)
N3—C17—C18—C19	179.41 (16)	C18—C17—N3—C23	−178.73 (17)
C22—C17—C18—C19	0.4 (2)	C22—C17—N3—C23	0.41 (16)
C17—C18—C19—C20	−0.1 (3)	C18—C17—N3—C16	6.5 (3)
C18—C19—C20—C21	−0.2 (3)	C22—C17—N3—C16	−174.36 (14)
N3—C17—C22—N4	−0.19 (17)	C15—C16—N3—C23	−85.09 (19)
C18—C17—C22—N4	179.06 (15)	C15—C16—N3—C17	88.61 (19)
N3—C17—C22—C21	−179.71 (14)	N3—C23—N4—C22	0.40 (18)
C18—C17—C22—C21	−0.5 (2)	C24—C23—N4—C22	−177.08 (16)
N4—C23—C24—C25	−3.0 (3)	C21—C22—N4—C23	179.34 (17)
N3—C23—C24—C25	179.75 (16)	C17—C22—N4—C23	−0.12 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12A···N1	0.97	2.61	2.999 (2)	105

Fig. 1


C19
C20
C18
C21
C22
C17
N4
C9
C8
O1
C16
N3
C23
N2
C7
C11
C13
C15
N1
C10
C12
C14
C24
C25
C1
C2
C6
C5
C3
C4