4-Chloro-*N*-methyl-6-(morpholin-4-yl)-*N*-phenyl-1,3,5-triazin-2-amine

Tao Zeng,* Wan-Zhong Ren and Lie-Gang Sun

Chemistry and Biology College, Yantai University, Yantai 264005, People's Republic of China
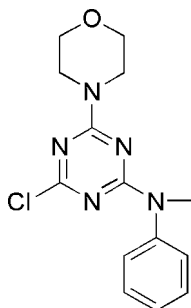
Correspondence e-mail: zengtaotj@126.com

In the title compound, $C_{14}H_{16}ClN_5O$, the phenyl and triazine rings form a dihedral angle of 69.34 (8)°. The morpholine ring adopts a chair conformation. The structure is stabilized by C—H$\cdots$N and intermolecular C—H$\cdots$O hydrogen-bonding interactions.

Related literature

For related literature, see: Cremer & Pople (1975); Dong *et al.* (2005); Manasek & Hrdlovik (1990); Mathias & Simanek (1994).

Experimental

Crystal data

$C_{14}H_{16}ClN_5O$	a = 17.121 (3) Å
M_r = 305.77	b = 17.308 (3) Å
Orthorhombic, $Pnna$	c = 10.0243 (17) Å
V = 2970.4 (9) Å^3	μ = 0.26 mm^{-1}
Z = 8	T = 294 (2) K
Mo $K\alpha$ radiation	0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	16109 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	3053 independent reflections
T_{min} = 0.944, T_{max} = 0.974	1607 reflections with $I > 2\sigma(I)$
	R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045	192 parameters
$wR(F^2)$ = 0.136	H-atom parameters constrained
S = 1.00	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
3053 reflections	$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C4—H4$A\cdots$N2	0.97	2.30	2.740 (3)	107
C7—H7$B\cdots$N3	0.97	2.35	2.782 (3)	106
C10—H10$\cdots$O1^i	0.93	2.44	3.327 (4)	158

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

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

References

Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Dong, C.-M., Chen, L.-G., Duan, X.-M., Shu, X.-G., Zeng, T. & Yan, X.-L. (2005). *Acta Cryst.* E**61**, o1168–o1169.

Manasek, Z. & Hrdlovik, P. (1990). European Patent EP 0377324.

Mathias, P. J. & Simanek, E. E. (1994). *J. Am. Chem. Soc.* **116**, 4326–4340.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supporting information

4-Chloro-*N*-methyl-6-(morpholin-4-yl)-*N*-phenyl-1,3,5-triazin-2-amine

Tao Zeng, Wan-Zhong Ren and Lie-Gang Sun

S1. Comment

2,4,6-Trichloro-1,3,5-triazine and its derivatives have been widely investigated, as a result of their importance as starting materials for many products. Moreover, these compounds possess valuable properties, as they are widely used as drugs and light stabilizers (Mathias & Simanek, 1994; Manasek & Hrdlovik, 1990). In the present paper, the crystal structure of the title compound, which has been synthesized from 2,4-dichloro-6-morpholin-4-yl-1,3,5-triazine and *N*-methylaniline, is reported.

In the title compound bond lengths and angles are within normal ranges (Table 1). The morpholine ring adopts a chair conformation with puckering parameters (Cremer and Pople, 1975) $Q = 0.549$ (2) Å, $\theta = 178.6$ (2)° and $\varphi = 121$ (12)°. The dihedral angle formed by the phenyl and triazine rings is 110.66 (8)°. The molecular conformation is stabilized by two intramolecular C—H···N hydrogen bonds (Table 2). In the crystal structure, the molecules are linked by intermolecular C—H···O hydrogen interactions (Table 2).

S2. Experimental

2,4-Dichloro-6-morpholino-1,3,5-triazine (11.75 g, 0.05 mol), which was prepared from morpholine and 2,4,6-tri-chloro-1,3,5-triazine according to the literature method (Dong *et al.*, 2005), and *N*-methylaniline (6.15 g, 0.05 mol) were dissolved in THF (60 ml) at 323 K with stirring for 2 h. A solution of Na_2CO_3 (2.76 g, 0.026 mol) in water (20 ml) was then added and the mixture stirred for a further 3 h. The solution was evaporated under reduced pressure and the precipitate was filtered off to give the title compound (12.69 g; yield 81.3%). Single crystals (m.p.371–372 K) suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate/ethanol (2:5 *v/v*) solution.

S3. Refinement

All the H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$ for methyl H atoms.
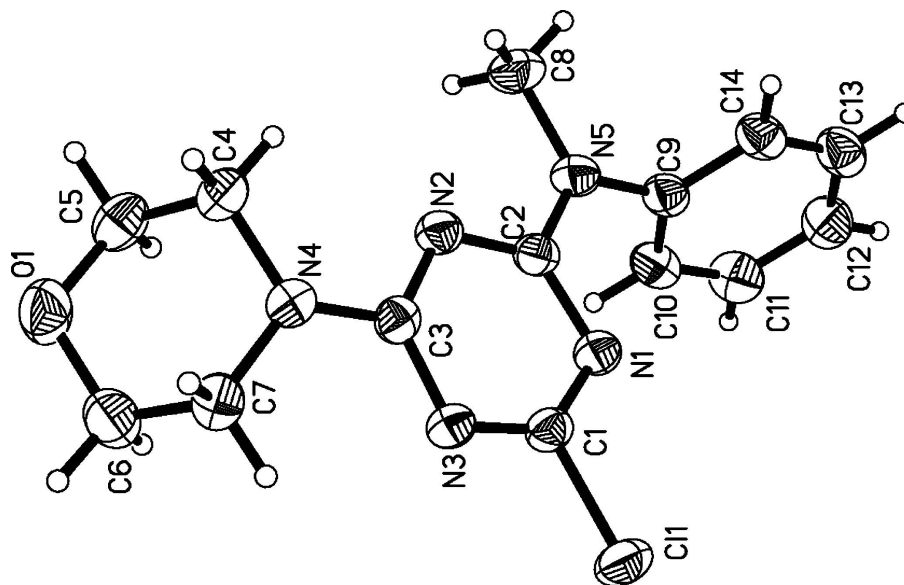
Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.
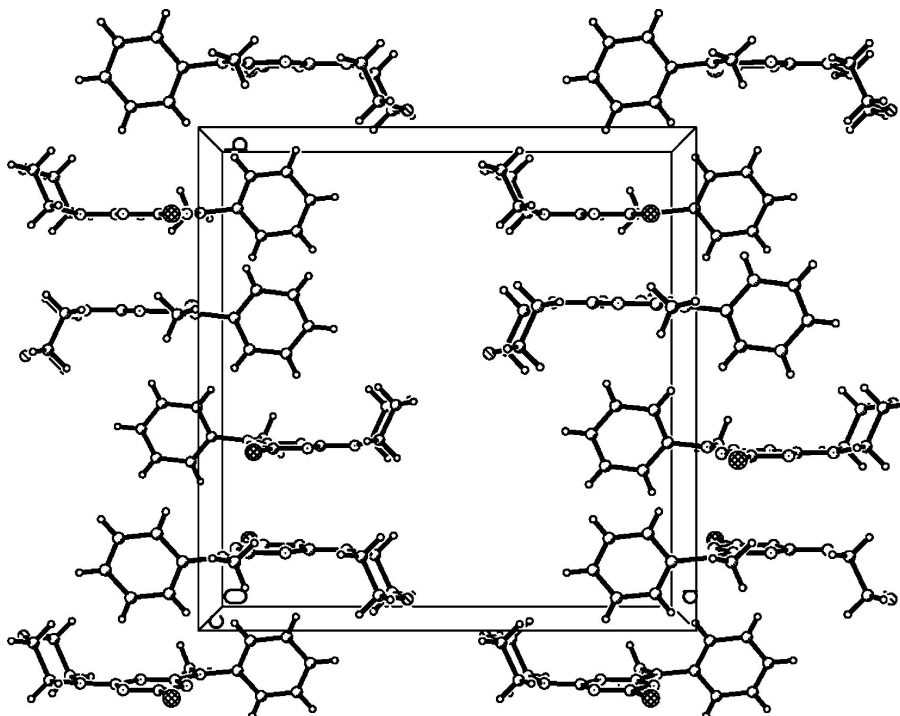
Figure 2

Packing diagram of the title compound viewed along the *c* axis.

4-Chloro-*N*-methyl-6-(morpholin-4-yl)-*N*-phenyl-1,3,5-triazin-2-amine

Crystal data

$C_{14}H_{16}ClN_5O$	$F(000) = 1280$
$M_r = 305.77$	$D_x = 1.367$ Mg m^{-3}
Orthorhombic, *Pnna*	Mo *Kα* radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2a 2bc	Cell parameters from 2473 reflections
$a = 17.121$ (3) Å	$\theta = 2.4$–22.2°
$b = 17.308$ (3) Å	$\mu = 0.26$ mm^{-1}
$c = 10.0243$ (17) Å	$T = 294$ K
$V = 2970.4$ (9) Å^3	Block, colourless
$Z = 8$	$0.22 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	16109 measured reflections
Radiation source: fine-focus sealed tube	3053 independent reflections
Graphite monochromator	1607 reflections with $I > 2\sigma(I)$
φ and *ω* scans	$R_{int} = 0.065$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 26.4°$, $\theta_{min} = 2.4°$
	$h = -21 \rightarrow 14$
	$k = -21 \rightarrow 21$
$T_{min} = 0.944$, $T_{max} = 0.974$	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.2969P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	
3053 reflections	$(\Delta/\sigma)_{max} = 0.003$
192 parameters	$\Delta\rho_{max} = 0.19$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: *SHELXL97* (Sheldrick, 1997), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0011 (3)

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}
Cl1	0.07523 (4)	0.34130 (5)	1.13890 (7)	0.0763 (3)
O1	0.41747 (12)	0.45017 (12)	0.7735 (2)	0.0843 (7)
N1	0.05798 (12)	0.35026 (11)	0.8833 (2)	0.0534 (6)

N2	0.16659 (12)	0.35391 (11)	0.73300 (19)	0.0518 (5)
N3	0.18823 (13)	0.34704 (11)	0.96853 (19)	0.0523 (5)
N4	0.29091 (13)	0.35119 (12)	0.8197 (2)	0.0582 (6)
N5	0.04129 (13)	0.36020 (12)	0.65470 (19)	0.0570 (6)
C1	0.11173 (16)	0.34659 (14)	0.9766 (2)	0.0510 (6)
C2	0.09049 (15)	0.35471 (13)	0.7589 (2)	0.0491 (6)
C3	0.21311 (15)	0.35082 (13)	0.8403 (2)	0.0481 (6)
C4	0.32424 (16)	0.35968 (16)	0.6869 (3)	0.0645 (8)
H4A	0.2837	0.3533	0.6202	0.077*
H4B	0.3635	0.3202	0.6724	0.077*
C5	0.36033 (17)	0.43769 (17)	0.6733 (3)	0.0701 (8)
H5A	0.3844	0.4423	0.5861	0.084*
H5B	0.3201	0.4769	0.6802	0.084*
C6	0.38457 (18)	0.44244 (18)	0.9033 (3)	0.0780 (9)
H6A	0.3455	0.4823	0.9161	0.094*
H6B	0.4252	0.4501	0.9694	0.094*
C7	0.34768 (15)	0.36491 (15)	0.9247 (3)	0.0602 (7)
H7A	0.3874	0.3250	0.9230	0.072*
H7B	0.3221	0.3635	1.0110	0.072*
C8	0.07219 (18)	0.36424 (18)	0.5184 (3)	0.0752 (9)
H8A	0.0936	0.4147	0.5027	0.113*
H8B	0.0308	0.3546	0.4559	0.113*
H8C	0.1124	0.3261	0.5073	0.113*
C9	−0.04133 (16)	0.36926 (16)	0.6715 (2)	0.0551 (7)
C10	−0.07178 (18)	0.43669 (17)	0.7235 (3)	0.0662 (8)
H10	−0.0386	0.4762	0.7509	0.079*
C11	−0.15150 (19)	0.44530 (19)	0.7346 (3)	0.0780 (9)
H11	−0.1721	0.4905	0.7703	0.094*
C12	−0.20090 (18)	0.3871 (2)	0.6931 (3)	0.0766 (9)
H12	−0.2547	0.3929	0.7009	0.092*
C13	−0.17014 (19)	0.32093 (18)	0.6404 (3)	0.0698 (8)
H13	−0.2034	0.2819	0.6116	0.084*
C14	−0.09104 (17)	0.31129 (16)	0.6294 (3)	0.0609 (7)
H14	−0.0708	0.2659	0.5937	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0725 (5)	0.1138 (7)	0.0427 (4)	−0.0041 (4)	0.0069 (3)	0.0068 (4)
O1	0.0782 (14)	0.0923 (16)	0.0824 (15)	−0.0245 (12)	−0.0001 (13)	0.0206 (12)
N1	0.0602 (14)	0.0568 (14)	0.0432 (12)	−0.0043 (11)	−0.0018 (11)	0.0057 (10)
N2	0.0591 (14)	0.0527 (14)	0.0435 (12)	−0.0033 (11)	0.0008 (11)	0.0012 (9)
N3	0.0590 (15)	0.0578 (14)	0.0401 (12)	−0.0032 (11)	0.0019 (10)	0.0050 (10)
N4	0.0584 (15)	0.0670 (15)	0.0492 (13)	−0.0053 (12)	0.0052 (11)	−0.0005 (10)
N5	0.0653 (15)	0.0653 (15)	0.0405 (12)	−0.0033 (11)	−0.0040 (11)	0.0007 (10)
C1	0.0616 (19)	0.0485 (15)	0.0430 (14)	−0.0034 (13)	0.0038 (13)	0.0039 (12)
C2	0.0635 (18)	0.0423 (15)	0.0416 (14)	−0.0059 (12)	−0.0014 (13)	0.0013 (11)
C3	0.0541 (17)	0.0392 (15)	0.0511 (16)	−0.0017 (12)	0.0043 (13)	0.0019 (11)

C4	0.0618 (18)	0.072 (2)	0.0596 (17)	−0.0030 (15)	0.0131 (14)	−0.0008 (14)
C5	0.072 (2)	0.073 (2)	0.0651 (19)	0.0081 (17)	0.0117 (16)	0.0175 (15)
C6	0.079 (2)	0.079 (2)	0.076 (2)	−0.0142 (17)	−0.0108 (18)	0.0022 (17)
C7	0.0547 (16)	0.0635 (18)	0.0623 (18)	0.0032 (14)	−0.0021 (14)	0.0108 (13)
C8	0.085 (2)	0.097 (2)	0.0429 (15)	−0.0017 (17)	0.0013 (15)	−0.0017 (15)
C9	0.0629 (18)	0.0592 (18)	0.0432 (15)	−0.0050 (15)	−0.0104 (13)	0.0061 (12)
C10	0.076 (2)	0.0608 (19)	0.0621 (17)	−0.0039 (16)	−0.0125 (16)	−0.0028 (14)
C11	0.073 (2)	0.080 (2)	0.081 (2)	0.0114 (18)	−0.0085 (18)	−0.0052 (17)
C12	0.060 (2)	0.095 (3)	0.074 (2)	0.0002 (19)	−0.0110 (16)	0.0061 (19)
C13	0.077 (2)	0.070 (2)	0.0625 (18)	−0.0112 (16)	−0.0200 (16)	0.0075 (15)
C14	0.070 (2)	0.0589 (18)	0.0542 (16)	−0.0014 (15)	−0.0142 (14)	0.0037 (13)

Geometric parameters (Å, º)

Cl1—C1	1.745 (2)	C6—C7	1.498 (4)
O1—C5	1.419 (3)	C6—H6A	0.9700
O1—C6	1.424 (3)	C6—H6B	0.9700
N1—C1	1.314 (3)	C7—H7A	0.9700
N1—C2	1.368 (3)	C7—H7B	0.9700
N2—C2	1.328 (3)	C8—H8A	0.9600
N2—C3	1.339 (3)	C8—H8B	0.9600
N3—C1	1.312 (3)	C8—H8C	0.9600
N3—C3	1.356 (3)	C9—C10	1.380 (4)
N4—C3	1.348 (3)	C9—C14	1.382 (4)
N4—C7	1.452 (3)	C10—C11	1.377 (4)
N4—C4	1.456 (3)	C10—H10	0.9300
N5—C2	1.345 (3)	C11—C12	1.379 (4)
N5—C9	1.433 (3)	C11—H11	0.9300
N5—C8	1.467 (3)	C12—C13	1.367 (4)
C4—C5	1.491 (4)	C12—H12	0.9300
C4—H4A	0.9700	C13—C14	1.369 (4)
C4—H4B	0.9700	C13—H13	0.9300
C5—H5A	0.9700	C14—H14	0.9300
C5—H5B	0.9700		
C5—O1—C6	111.1 (2)	O1—C6—H6B	109.1
C1—N1—C2	111.5 (2)	C7—C6—H6B	109.1
C2—N2—C3	115.3 (2)	H6A—C6—H6B	107.8
C1—N3—C3	111.9 (2)	N4—C7—C6	109.0 (2)
C3—N4—C7	123.5 (2)	N4—C7—H7A	109.9
C3—N4—C4	121.8 (2)	C6—C7—H7A	109.9
C7—N4—C4	112.6 (2)	N4—C7—H7B	109.9
C2—N5—C9	122.3 (2)	C6—C7—H7B	109.9
C2—N5—C8	120.0 (2)	H7A—C7—H7B	108.3
C9—N5—C8	117.4 (2)	N5—C8—H8A	109.5
N3—C1—N1	130.9 (2)	N5—C8—H8B	109.5
N3—C1—Cl1	114.54 (19)	H8A—C8—H8B	109.5
N1—C1—Cl1	114.6 (2)	N5—C8—H8C	109.5

N2—C2—N5	117.6 (2)	H8A—C8—H8C	109.5
N2—C2—N1	125.2 (2)	H8B—C8—H8C	109.5
N5—C2—N1	117.2 (2)	C10—C9—C14	119.8 (3)
N2—C3—N4	117.7 (2)	C10—C9—N5	120.6 (3)
N2—C3—N3	125.2 (2)	C14—C9—N5	119.5 (3)
N4—C3—N3	117.1 (2)	C11—C10—C9	119.8 (3)
N4—C4—C5	109.7 (2)	C11—C10—H10	120.1
N4—C4—H4A	109.7	C9—C10—H10	120.1
C5—C4—H4A	109.7	C10—C11—C12	120.3 (3)
N4—C4—H4B	109.7	C10—C11—H11	119.9
C5—C4—H4B	109.7	C12—C11—H11	119.9
H4A—C4—H4B	108.2	C13—C12—C11	119.5 (3)
O1—C5—C4	111.0 (2)	C13—C12—H12	120.3
O1—C5—H5A	109.4	C11—C12—H12	120.3
C4—C5—H5A	109.4	C12—C13—C14	121.0 (3)
O1—C5—H5B	109.4	C12—C13—H13	119.5
C4—C5—H5B	109.4	C14—C13—H13	119.5
H5A—C5—H5B	108.0	C13—C14—C9	119.8 (3)
O1—C6—C7	112.4 (2)	C13—C14—H14	120.1
O1—C6—H6A	109.1	C9—C14—H14	120.1
C7—C6—H6A	109.1		
C3—N3—C1—N1	−1.1 (4)	C3—N4—C4—C5	108.2 (3)
C3—N3—C1—Cl1	179.70 (16)	C7—N4—C4—C5	−55.8 (3)
C2—N1—C1—N3	0.5 (4)	C6—O1—C5—C4	−58.0 (3)
C2—N1—C1—Cl1	179.67 (16)	N4—C4—C5—O1	56.6 (3)
C3—N2—C2—N5	178.0 (2)	C5—O1—C6—C7	57.5 (3)
C3—N2—C2—N1	−2.1 (3)	C3—N4—C7—C6	−109.5 (3)
C9—N5—C2—N2	−173.7 (2)	C4—N4—C7—C6	54.2 (3)
C8—N5—C2—N2	0.6 (3)	O1—C6—C7—N4	−54.6 (3)
C9—N5—C2—N1	6.4 (3)	C2—N5—C9—C10	68.3 (3)
C8—N5—C2—N1	−179.3 (2)	C8—N5—C9—C10	−106.2 (3)
C1—N1—C2—N2	1.3 (3)	C2—N5—C9—C14	−114.8 (3)
C1—N1—C2—N5	−178.8 (2)	C8—N5—C9—C14	70.8 (3)
C2—N2—C3—N4	−178.9 (2)	C14—C9—C10—C11	0.8 (4)
C2—N2—C3—N3	1.3 (3)	N5—C9—C10—C11	177.8 (2)
C7—N4—C3—N2	166.1 (2)	C9—C10—C11—C12	−0.5 (4)
C4—N4—C3—N2	3.9 (3)	C10—C11—C12—C13	−0.2 (5)
C7—N4—C3—N3	−14.1 (3)	C11—C12—C13—C14	0.6 (4)
C4—N4—C3—N3	−176.3 (2)	C12—C13—C14—C9	−0.3 (4)
C1—N3—C3—N2	0.1 (3)	C10—C9—C14—C13	−0.5 (4)
C1—N3—C3—N4	−179.6 (2)	N5—C9—C14—C13	−177.4 (2)

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C4—H4A⋯N2	0.97	2.30	2.740 (3)	107

C7—H7*B*···N3	0.97	2.35	2.782 (3)	106
C10—H10···O1^i	0.93	2.44	3.327 (4)	158

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