Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,6-Dimorpholino-*N*-(2,4,4-trimethylpentan-2-yl)-1,3,5-triazin-2-amine

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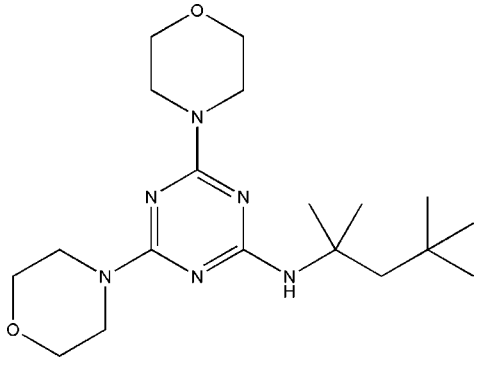
Received 2 September 2007; accepted 5 September 2007

Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.103; data-to-parameter ratio = 14.4.

In the title compound, $C_{19}H_{34}N_6O_2$, both morpholine rings adopt chair conformations. In the crystal structure, N—H···N hydrogen bonds link the molecules into chains along c.

Related literature

For the preparation and uses of the title compound and similar compounds, see: Borzatta & Carrozza (1991); Deng *et al.* (2006); Kaiser & Thurston (1951).



Experimental

Crystal data

$C_{19}H_{34}N_6O_2$
M_r = 378.52
Monoclinic, $P2_1/c$
a = 10.247 (2) Å
b = 16.718 (3) Å
c = 12.107 (2) Å
β = 94.82 (3)°
V = 2066.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 113 (2) K
0.08 × 0.08 × 0.02 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.984, T_{max} = 0.998
20763 measured reflections
3641 independent reflections
3159 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.09
3641 reflections
253 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6*C*···N1^{i}	0.885 (8)	2.392 (9)	3.2715 (15)	172.4 (11)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2350).

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  doi:10.1107/S1600536807043462

supplementary materials

Acta Cryst. (2007). E**63**, o4028 [**doi:10.1107/S1600536807043462**]

4,6-Dimorpholino-*N*-(2,4,4-trimethylpentan-2-yl)-1,3,5-triazin-2-amine

J.-Y. Dong and P.-M. Huang

Comment

The title compound (I) is an important intermediate in the preparation of hindered light stabilizers(Borzatta & Carrozza, 1991). Compounds containing a triazine ring are widely used in polymers, dyes, drugs and hindered amine light stabilizers (Deng *et al.*, 2006). We report here the crystal structure of the title compound (I) (Fig. 1). In (I) both morpholine rings adopt a chair conformation and the triazine ring is essentially planar with an r.m.s. deviation from the mean plane of 0.0105 Å. In the crystal N6—H6C···N1 hydrogen bonds link the molecules into chains along c, Table 1.

Experimental

The title compound was prepared according to the method of Kaiser & Thurston (1951) in 71% yield. Crystals of (I) were obtained by slow evaporation of a solution in methanol (m.p. 431–433 K).

Refinement

The amine H atom was located in a Fourier map and was refined freely with an isotropic displacement parameter. All other H atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.97 Å, $U_{iso} = 1.2U_{eq}$ (C) for CH_2 and 0.96 Å, $U_{iso} = 1.5U_{eq}$ (C) for CH_3 atoms.

Figures

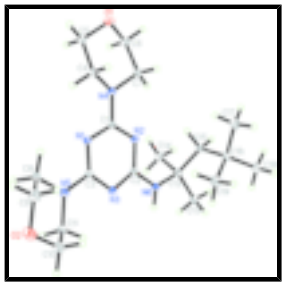


Fig. 1. A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

4,6-Dimorpholino-*N*-(2,4,4-trimethylpentan-2-yl)-1,3,5-triazin-2-amine

Crystal data

$C_{19}H_{34}N_6O_2$	F_{000} = 824
M_r = 378.52	D_x = 1.217 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 431-433 K K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å

a = 10.247 (2) Å	Cell parameters from 5929 reflections
b = 16.718 (3) Å	θ = 2.1–27.9º
c = 12.107 (2) Å	μ = 0.08 mm^{-1}
β = 94.82 (3)º	T = 113 (2) K
V = 2066.6 (7) $Å^3$	Block, colorless
Z = 4	0.08 × 0.08 × 0.02 mm

Data collection

Rigaku Saturn CCD diffractometer	3641 independent reflections
Radiation source: rotating anode	3159 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.034
T = 113(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	$h = -12 \rightarrow 12$
T_{min} = 0.984, T_{max} = 0.998	$k = -18 \rightarrow 19$
20763 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.103	$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.0832P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max}$ = <0.001
3641 reflections	$\Delta\rho_{max}$ = 0.20 e $Å^{-3}$
253 parameters	$\Delta\rho_{min}$ = −0.27 e $Å^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
O1	0.82017 (9)	0.02524 (5)	0.97507 (7)	0.0292 (2)
O2	0.14099 (9)	0.33956 (6)	0.65039 (9)	0.0375 (3)
N1	0.55524 (10)	0.20367 (6)	0.72321 (8)	0.0181 (2)
N2	0.70950 (10)	0.14783 (6)	0.60724 (8)	0.0173 (2)
N3	0.54840 (9)	0.24124 (6)	0.53212 (8)	0.0170 (2)
N4	0.70730 (10)	0.11069 (6)	0.79018 (8)	0.0203 (2)
N5	0.40537 (10)	0.29537 (6)	0.64901 (8)	0.0235 (3)
N6	0.69655 (10)	0.18699 (6)	0.42305 (8)	0.0173 (2)
C1	0.65477 (11)	0.15522 (7)	0.70307 (9)	0.0166 (3)
C2	0.65151 (11)	0.19201 (7)	0.52442 (9)	0.0156 (3)
C3	0.50656 (11)	0.24526 (7)	0.63360 (9)	0.0165 (3)
C4	0.63464 (13)	0.09771 (7)	0.88701 (10)	0.0218 (3)
H4A	0.5807	0.0502	0.8762	0.026*
H4B	0.5775	0.1429	0.8968	0.026*
C5	0.72851 (14)	0.08778 (8)	0.98842 (10)	0.0273 (3)
H5A	0.7754	0.1375	1.0033	0.033*
H5B	0.6796	0.0760	1.0517	0.033*
C6	0.89372 (13)	0.04203 (8)	0.88310 (11)	0.0275 (3)
H6A	0.9564	−0.0007	0.8754	0.033*
H6B	0.9423	0.0913	0.8971	0.033*
C7	0.80720 (12)	0.05017 (7)	0.77602 (10)	0.0227 (3)
H7A	0.8596	0.0657	0.7165	0.027*
H7B	0.7659	−0.0007	0.7568	0.027*
C8	0.34451 (13)	0.30169 (8)	0.75292 (11)	0.0275 (3)
H8A	0.3591	0.3547	0.7840	0.033*
H8B	0.3832	0.2630	0.8056	0.033*
C9	0.19977 (14)	0.28629 (9)	0.73206 (13)	0.0362 (4)
H9A	0.1857	0.2315	0.7073	0.043*
H9B	0.1584	0.2930	0.8006	0.043*
C10	0.19844 (13)	0.32924 (9)	0.54852 (12)	0.0308 (3)
H10A	0.1570	0.3654	0.4936	0.037*
H10B	0.1828	0.2750	0.5222	0.037*
C11	0.34334 (12)	0.34494 (8)	0.56048 (10)	0.0233 (3)
H11A	0.3806	0.3328	0.4913	0.028*
H11B	0.3594	0.4010	0.5775	0.028*
C12	0.81655 (11)	0.14606 (7)	0.39230 (10)	0.0191 (3)
C13	0.82342 (13)	0.16201 (8)	0.26896 (10)	0.0254 (3)
H13A	0.7446	0.1432	0.2287	0.038*
H13B	0.8974	0.1344	0.2435	0.038*
H13C	0.8325	0.2184	0.2569	0.038*
C14	0.93531 (12)	0.18489 (8)	0.45587 (11)	0.0267 (3)
H14A	0.9350	0.2413	0.4411	0.040*
H14B	1.0141	0.1616	0.4326	0.040*
H14C	0.9314	0.1762	0.5339	0.040*
C15	0.81944 (12)	0.05571 (7)	0.42141 (10)	0.0195 (3)

H15A	0.9057	0.0364	0.4071	0.023*
H15B	0.8142	0.0521	0.5009	0.023*
C16	0.71964 (12)	−0.00559 (7)	0.36787 (10)	0.0236 (3)
C17	0.71755 (15)	−0.07566 (8)	0.44923 (12)	0.0337 (3)
H17A	0.6604	−0.1167	0.4178	0.051*
H17B	0.6864	−0.0574	0.5174	0.051*
H17C	0.8045	−0.0968	0.4634	0.051*
C18	0.76316 (15)	−0.03851 (8)	0.25880 (11)	0.0345 (4)
H18A	0.7000	−0.0767	0.2284	0.052*
H18B	0.8468	−0.0641	0.2724	0.052*
H18C	0.7700	0.0046	0.2072	0.052*
C19	0.58034 (13)	0.02736 (8)	0.34862 (12)	0.0323 (3)
H19A	0.5780	0.0686	0.2933	0.048*
H19B	0.5539	0.0492	0.4166	0.048*
H19C	0.5217	−0.0150	0.3239	0.048*
H6C	0.6524 (12)	0.2176 (7)	0.3734 (9)	0.022 (3)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0367 (5)	0.0304 (5)	0.0197 (5)	0.0065 (4)	−0.0024 (4)	0.0063 (4)
O2	0.0223 (5)	0.0435 (6)	0.0477 (7)	0.0075 (4)	0.0092 (5)	0.0084 (5)
N1	0.0206 (5)	0.0188 (5)	0.0151 (5)	0.0024 (4)	0.0018 (4)	0.0003 (4)
N2	0.0190 (5)	0.0187 (5)	0.0142 (5)	0.0010 (4)	0.0009 (4)	0.0005 (4)
N3	0.0170 (5)	0.0180 (5)	0.0161 (5)	0.0004 (4)	0.0014 (4)	0.0006 (4)
N4	0.0236 (6)	0.0220 (5)	0.0152 (5)	0.0047 (4)	0.0016 (4)	0.0023 (4)
N5	0.0224 (6)	0.0300 (6)	0.0186 (6)	0.0097 (5)	0.0054 (4)	0.0041 (4)
N6	0.0194 (5)	0.0192 (5)	0.0134 (5)	0.0038 (4)	0.0022 (4)	0.0024 (4)
C1	0.0186 (6)	0.0163 (6)	0.0148 (6)	−0.0019 (5)	−0.0004 (5)	−0.0009 (5)
C2	0.0160 (6)	0.0149 (6)	0.0157 (6)	−0.0029 (5)	0.0004 (5)	−0.0005 (5)
C3	0.0161 (6)	0.0170 (6)	0.0165 (6)	−0.0018 (5)	0.0013 (5)	−0.0008 (5)
C4	0.0286 (7)	0.0219 (7)	0.0152 (6)	0.0022 (5)	0.0041 (5)	0.0010 (5)
C5	0.0391 (8)	0.0251 (7)	0.0171 (7)	0.0033 (6)	−0.0005 (6)	−0.0001 (5)
C6	0.0266 (7)	0.0298 (7)	0.0253 (7)	0.0025 (6)	−0.0018 (6)	0.0052 (6)
C7	0.0244 (7)	0.0234 (7)	0.0203 (7)	0.0051 (5)	0.0010 (5)	0.0010 (5)
C8	0.0304 (7)	0.0301 (7)	0.0235 (7)	0.0097 (6)	0.0103 (6)	0.0011 (6)
C9	0.0323 (8)	0.0360 (8)	0.0425 (9)	0.0045 (6)	0.0165 (7)	0.0083 (7)
C10	0.0254 (7)	0.0312 (8)	0.0348 (8)	0.0023 (6)	−0.0029 (6)	−0.0010 (6)
C11	0.0239 (7)	0.0227 (7)	0.0234 (7)	0.0063 (5)	0.0021 (5)	0.0031 (5)
C12	0.0177 (6)	0.0215 (6)	0.0185 (6)	0.0022 (5)	0.0042 (5)	0.0006 (5)
C13	0.0288 (7)	0.0270 (7)	0.0216 (7)	0.0064 (6)	0.0092 (6)	0.0039 (5)
C14	0.0219 (7)	0.0275 (7)	0.0310 (8)	−0.0024 (5)	0.0045 (6)	−0.0004 (6)
C15	0.0191 (6)	0.0221 (7)	0.0174 (6)	0.0055 (5)	0.0019 (5)	0.0013 (5)
C16	0.0254 (7)	0.0208 (7)	0.0244 (7)	0.0017 (5)	0.0007 (5)	−0.0013 (5)
C17	0.0368 (8)	0.0246 (7)	0.0401 (9)	−0.0019 (6)	0.0057 (7)	0.0036 (6)
C18	0.0476 (9)	0.0275 (8)	0.0275 (8)	0.0046 (7)	−0.0013 (7)	−0.0063 (6)
C19	0.0253 (7)	0.0275 (8)	0.0428 (9)	−0.0029 (6)	−0.0048 (6)	−0.0058 (6)

Geometric parameters (Å, °)

O1—C5	1.4237 (16)	C9—H9A	0.9700
O1—C6	1.4239 (16)	C9—H9B	0.9700
O2—C10	1.4211 (17)	C10—C11	1.5027 (18)
O2—C9	1.4259 (17)	C10—H10A	0.9700
N1—C1	1.3407 (15)	C10—H10B	0.9700
N1—C3	1.3484 (15)	C11—H11A	0.9700
N2—C1	1.3360 (15)	C11—H11B	0.9700
N2—C2	1.3430 (15)	C12—C13	1.5243 (17)
N3—C3	1.3366 (15)	C12—C14	1.5287 (18)
N3—C2	1.3487 (15)	C12—C15	1.5508 (17)
N4—C1	1.3641 (15)	C13—H13A	0.9600
N4—C4	1.4569 (15)	C13—H13B	0.9600
N4—C7	1.4596 (16)	C13—H13C	0.9600
N5—C3	1.3580 (16)	C14—H14A	0.9600
N5—C8	1.4541 (16)	C14—H14B	0.9600
N5—C11	1.4577 (16)	C14—H14C	0.9600
N6—C2	1.3496 (15)	C15—C16	1.5507 (18)
N6—C12	1.4818 (15)	C15—H15A	0.9700
N6—H6C	0.885 (8)	C15—H15B	0.9700
C4—C5	1.5039 (18)	C16—C19	1.5295 (18)
C4—H4A	0.9700	C16—C18	1.5311 (18)
C4—H4B	0.9700	C16—C17	1.5318 (18)
C5—H5A	0.9700	C17—H17A	0.9600
C5—H5B	0.9700	C17—H17B	0.9600
C6—C7	1.5138 (18)	C17—H17C	0.9600
C6—H6A	0.9700	C18—H18A	0.9600
C6—H6B	0.9700	C18—H18B	0.9600
C7—H7A	0.9700	C18—H18C	0.9600
C7—H7B	0.9700	C19—H19A	0.9600
C8—C9	1.506 (2)	C19—H19B	0.9600
C8—H8A	0.9700	C19—H19C	0.9600
C8—H8B	0.9700		
C5—O1—C6	109.97 (9)	O2—C10—H10A	109.2
C10—O2—C9	110.15 (10)	C11—C10—H10A	109.2
C1—N1—C3	113.63 (10)	O2—C10—H10B	109.2
C1—N2—C2	113.95 (10)	C11—C10—H10B	109.2
C3—N3—C2	114.07 (10)	H10A—C10—H10B	107.9
C1—N4—C4	120.55 (10)	N5—C11—C10	109.74 (11)
C1—N4—C7	121.50 (10)	N5—C11—H11A	109.7
C4—N4—C7	113.71 (10)	C10—C11—H11A	109.7
C3—N5—C8	123.48 (10)	N5—C11—H11B	109.7
C3—N5—C11	122.71 (10)	C10—C11—H11B	109.7
C8—N5—C11	113.74 (10)	H11A—C11—H11B	108.2
C2—N6—C12	127.71 (10)	N6—C12—C13	105.85 (10)
C2—N6—H6C	112.8 (8)	N6—C12—C14	108.64 (10)
C12—N6—H6C	119.0 (8)	C13—C12—C14	108.58 (10)

N2—C1—N1	126.51 (11)	N6—C12—C15	113.14 (9)
N2—C1—N4	116.99 (10)	C13—C12—C15	113.04 (10)
N1—C1—N4	116.47 (10)	C14—C12—C15	107.45 (10)
N2—C2—N3	125.73 (10)	C12—C13—H13A	109.5
N2—C2—N6	118.76 (10)	C12—C13—H13B	109.5
N3—C2—N6	115.50 (10)	H13A—C13—H13B	109.5
N3—C3—N1	126.02 (11)	C12—C13—H13C	109.5
N3—C3—N5	117.71 (11)	H13A—C13—H13C	109.5
N1—C3—N5	116.27 (10)	H13B—C13—H13C	109.5
N4—C4—C5	109.77 (11)	C12—C14—H14A	109.5
N4—C4—H4A	109.7	C12—C14—H14B	109.5
C5—C4—H4A	109.7	H14A—C14—H14B	109.5
N4—C4—H4B	109.7	C12—C14—H14C	109.5
C5—C4—H4B	109.7	H14A—C14—H14C	109.5
H4A—C4—H4B	108.2	H14B—C14—H14C	109.5
O1—C5—C4	111.79 (10)	C16—C15—C12	123.32 (10)
O1—C5—H5A	109.3	C16—C15—H15A	106.5
C4—C5—H5A	109.3	C12—C15—H15A	106.5
O1—C5—H5B	109.3	C16—C15—H15B	106.5
C4—C5—H5B	109.3	C12—C15—H15B	106.5
H5A—C5—H5B	107.9	H15A—C15—H15B	106.5
O1—C6—C7	112.15 (11)	C19—C16—C18	109.50 (11)
O1—C6—H6A	109.2	C19—C16—C17	108.06 (11)
C7—C6—H6A	109.2	C18—C16—C17	107.49 (11)
O1—C6—H6B	109.2	C19—C16—C15	113.57 (10)
C7—C6—H6B	109.2	C18—C16—C15	111.62 (11)
H6A—C6—H6B	107.9	C17—C16—C15	106.32 (11)
N4—C7—C6	109.13 (10)	C16—C17—H17A	109.5
N4—C7—H7A	109.9	C16—C17—H17B	109.5
C6—C7—H7A	109.9	H17A—C17—H17B	109.5
N4—C7—H7B	109.9	C16—C17—H17C	109.5
C6—C7—H7B	109.9	H17A—C17—H17C	109.5
H7A—C7—H7B	108.3	H17B—C17—H17C	109.5
N5—C8—C9	109.31 (12)	C16—C18—H18A	109.5
N5—C8—H8A	109.8	C16—C18—H18B	109.5
C9—C8—H8A	109.8	H18A—C18—H18B	109.5
N5—C8—H8B	109.8	C16—C18—H18C	109.5
C9—C8—H8B	109.8	H18A—C18—H18C	109.5
H8A—C8—H8B	108.3	H18B—C18—H18C	109.5
O2—C9—C8	111.24 (11)	C16—C19—H19A	109.5
O2—C9—H9A	109.4	C16—C19—H19B	109.5
C8—C9—H9A	109.4	H19A—C19—H19B	109.5
O2—C9—H9B	109.4	C16—C19—H19C	109.5
C8—C9—H9B	109.4	H19A—C19—H19C	109.5
H9A—C9—H9B	108.0	H19B—C19—H19C	109.5
O2—C10—C11	111.91 (11)		
C2—N2—C1—N1	−3.13 (17)	C6—O1—C5—C4	59.52 (14)
C2—N2—C1—N4	178.72 (10)	N4—C4—C5—O1	−55.56 (14)
C3—N1—C1—N2	2.64 (16)	C5—O1—C6—C7	−59.49 (14)

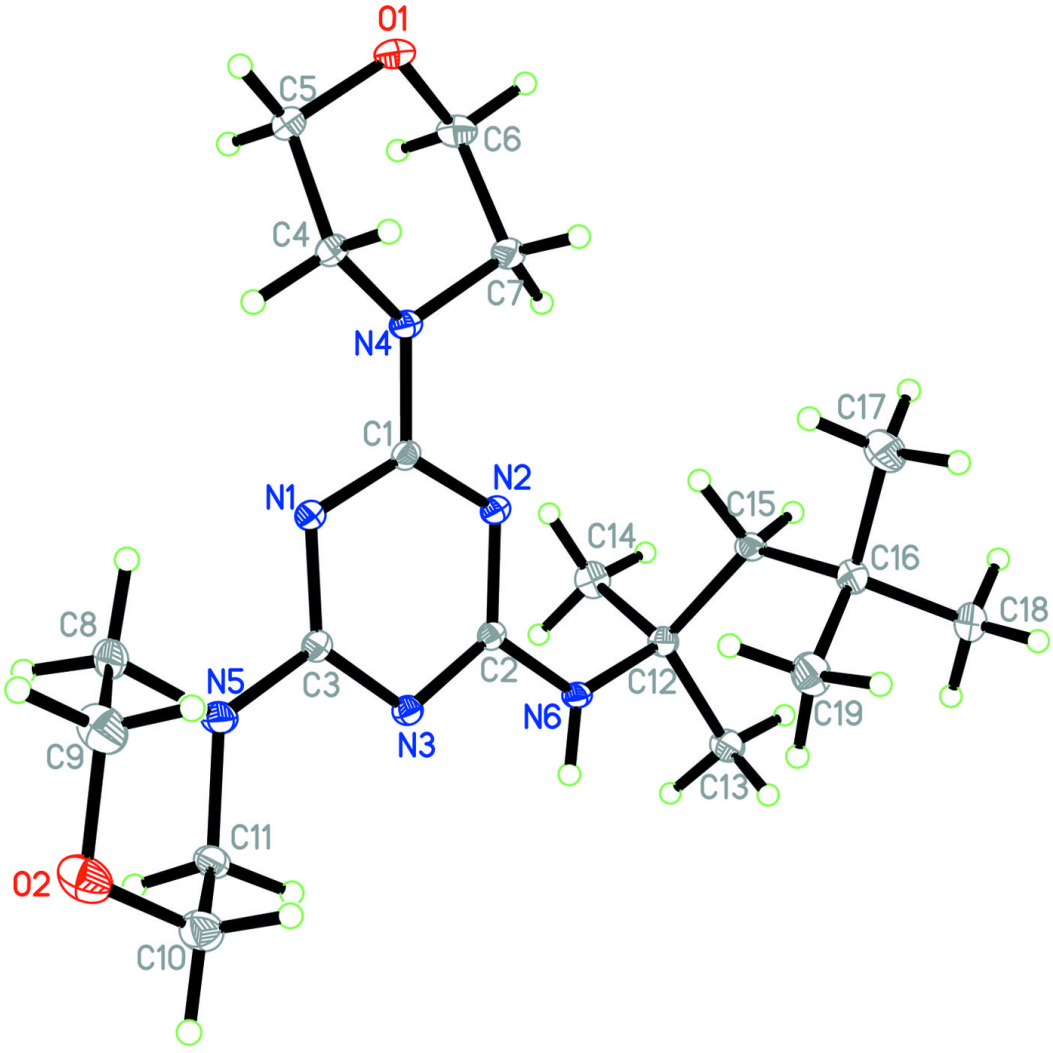
C3—N1—C1—N4	−179.21 (10)	C1—N4—C7—C6	150.99 (11)
C4—N4—C1—N2	−163.16 (10)	C4—N4—C7—C6	−52.03 (14)
C7—N4—C1—N2	−7.73 (16)	O1—C6—C7—N4	55.05 (14)
C4—N4—C1—N1	18.50 (16)	C3—N5—C8—C9	−124.15 (13)
C7—N4—C1—N1	173.93 (10)	C11—N5—C8—C9	52.85 (15)
C1—N2—C2—N3	0.82 (16)	C10—O2—C9—C8	60.37 (15)
C1—N2—C2—N6	−177.92 (10)	N5—C8—C9—O2	−56.35 (15)
C3—N3—C2—N2	1.58 (16)	C9—O2—C10—C11	−59.46 (15)
C3—N3—C2—N6	−179.64 (10)	C3—N5—C11—C10	125.17 (13)
C12—N6—C2—N2	−9.04 (17)	C8—N5—C11—C10	−51.86 (15)
C12—N6—C2—N3	172.09 (10)	O2—C10—C11—N5	54.40 (14)
C2—N3—C3—N1	−2.16 (16)	C2—N6—C12—C13	−177.64 (11)
C2—N3—C3—N5	178.14 (10)	C2—N6—C12—C14	−61.20 (15)
C1—N1—C3—N3	0.26 (16)	C2—N6—C12—C15	58.04 (15)
C1—N1—C3—N5	179.96 (10)	N6—C12—C15—C16	63.93 (15)
C8—N5—C3—N3	175.78 (11)	C13—C12—C15—C16	−56.37 (15)
C11—N5—C3—N3	−0.96 (17)	C14—C12—C15—C16	−176.15 (11)
C8—N5—C3—N1	−3.95 (17)	C12—C15—C16—C19	−37.84 (16)
C11—N5—C3—N1	179.31 (11)	C12—C15—C16—C18	86.53 (14)
C1—N4—C4—C5	−150.20 (11)	C12—C15—C16—C17	−156.54 (11)
C7—N4—C4—C5	52.59 (13)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6C···N1^{i}	0.885 (8)	2.392 (9)	3.2715 (15)	172.4 (11)

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

Fig. 1


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