Two polymorphs of N,N′-diphenyl-2-[1-(propyl-amino)ethylidene]propanediamide

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Two polymorphs of the title compound, $C_{20}H_{23}N_3O_2$, have been isolated. Polymorph (**I**) crystallizes in the monoclinic space group $P2_1/n$ and polymorph (**II**) in the tetragonal space group $I4_1/a$. The main difference between the two polymorphs on the molecular level is the orientation of the *n*-propyl group. This group is antiperiplanar in (**I**) and synclinal in (**II**). The core of the molecule consists of two carbamoyl units bound to an enamine unit. The most prominent features are intramolecular N—H⋯O hydrogen bonds in both polymorphs. Both polymorphs form dimers with graph set $R_2^2(12)$ *via* intermolecular N—H⋯O hydrogen bonds. Adjacent dimers of (**I**) are connected *via* a weak C—H⋯O interaction, resulting in a chain parallel to the crystallographic *a*-axis. The dimers of (**II**) are connected by weak C—H⋯π interactions, forming intermolecular chains along the *c*-axis direction.

1. Chemical context

N,*N*′-Diphenyl-2-[1-(propylamino)ethylidene]propanedi-amide is an insertion product from an enamine and phenyl isocyanate. This was obtained in our work with different types of silicon–nitrogen compounds (Herbig *et al.*, 2019*a*, 2021, 2022). The Si—N bonds can be subjected to insertion of different heteroallenes such as CO_2 and isocyanates (Kraushaar *et al.*, 2012, 2014, 2017; Herbig *et al.*, 2018, 2019*b*). Insertion reactions into silicon-substituted enamines were investigated as a continuation of our research in this area.
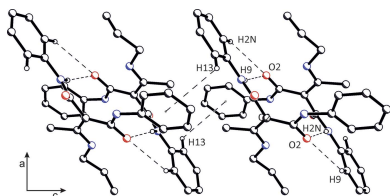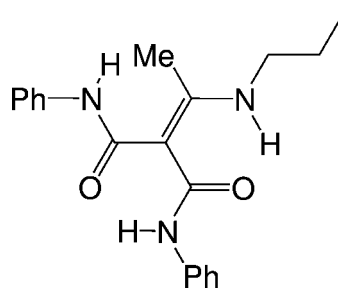
2. Structural commentary

Two polymorphs of the title compound were obtained from a single reaction batch. Polymorph (**I**) crystallizes in the monoclinic space group $P2_1/n$, polymorph (**II**) in the tetragonal space group $I4_1/a$. The main difference between the polymorphs on the molecular level is the orientation of the *n*-propyl group. This group is antiperiplanar in (**I**) and synclinal in (**II**), as can be seen from the values of the torsion angles C1—C2—C3—N1 (see Tables 1, 2 and Figs. 1, 2). The *n*-propyl

Table 1
Selected geometric parameters (Å, °) for (I).

N1—C4	1.331 (2)	C7—N2	1.364 (2)
C4—C5	1.400 (2)	C14—O2	1.254 (2)
C7—O1	1.237 (2)	C14—N3	1.360 (2)
C1—C2—C3—N1	−169.39 (17)		

Table 2
Selected geometric parameters (Å, °) for (II).

N1—C4	1.331 (3)	C7—N2	1.369 (3)
C4—C5	1.394 (3)	C14—O2	1.257 (2)
C7—O1	1.234 (2)	C14—N3	1.366 (2)
C1A—C2A—C3A—N1	65.0 (4)	C1B—C2B—C3B—N1	−46 (2)

group with C1—C2—C3 is disordered in (**II**), with site occupancies of 0.794 (7) and 0.206 (7) for parts A and B, respectively.

The double bond between C4 and C5 is slightly elongated [1.400 (2) and 1.394 (3) Å], but not as strongly as in the push–pull alkenes from cyclic ketene-N,N'-acetals, which have values of 1.45 to 1.47 Å (Ye *et al.*, 2010). The carbamoyl units are characterized by C=O double bonds and shortened C—N bonds (Tables 1 and 2), the latter having values between 1.360 (2) to 1.369 (3) Å, whereas the sum of covalent radii of C and N is 1.472 Å (Pauling, 1962).

The core of the molecule consists of two carbamoyl units (N2—C7—O1 and N3—C14—O2) bound to an enamine unit (C5—C4—N1). These planar units span certain dihedral angles between each other. The dihedral angles are listed in Table 3. The dihedral angle between N1—C4—C5 and N3—C14—O2 is small in both polymorphs, with values of 10.1 (4)° in (**I**) and 8.0 (3)° in (**II**). The dihedral angles between plane N1—C4—C5 and plane N2—C7—O1 adopt larger values of 49.0 (2)° in (**I**) and 51.5 (2)° in (**II**). This means that the

Table 3
Dihedral angles (°) between selected planes in (I) and (II).

Plane 1	Plane 2	(**I**)	(**II**)
N1/C4/C5	N3/C14/O2	10.1 (4)	8.0 (3)
N1/C4/C5	N2/C7/O1	49.0 (2)	51.5 (3)
N2/C7/O1	phenyl C8–C13	26.8 (2)	23.6 (2)
N3/C14/O2	phenyl C15–C20	17.1 (3)	10.4 (2)

carbamoyl unit N2—C7—O1 is rotated further away from the enamine group than the other carbamoyl unit. Small differences between both polymorphs are found in the orientation of the phenyl groups relative to the carbamoyl units (see Table 3).

There are several intramolecular hydrogen bonds in (**I**) and (**II**). The interactions N1—H1N···O2 and N3—H3N···O1 feature H···O distances below 2 Å (see Tables 4 and 5), which qualifies these as hydrogen bonds of moderate strength (Gilli & Gilli, 2009). Further intramolecular interactions are present between C6—H6B···N2, C13—H13···O1, and C20—H20···O2 in both polymorphs.

3. Supramolecular features

The density of (**I**) is 1.243 and of (**II**) 1.235 Mg m^{-3}. The molecular arrangement is different in both crystals because of the crystal symmetry. The 2_1 screw axes running parallel to the b-axis in the monoclinic crystal (**I**) lead to a parallel arrangement of molecules in the unit cell. In contrast, in the tetragonal crystal of (**II**), the molecules are grouped around the 4_1 screw axes running parallel to the c-axis. This leads to pairs of molecules that are oriented at an angle of 90° to each other. In (**I**) and (**II**), these dimers are formed by the intermolecular N2—H2N···O2 hydrogen bonds, described by graph set $R_2^2(12)$ (see Fig. 3). Adjacent dimers are connected

Figure 1
Diagram of polymorph (**I**) showing the atom-labelling scheme. Atomic displacement parameters are at the 50% probability level.
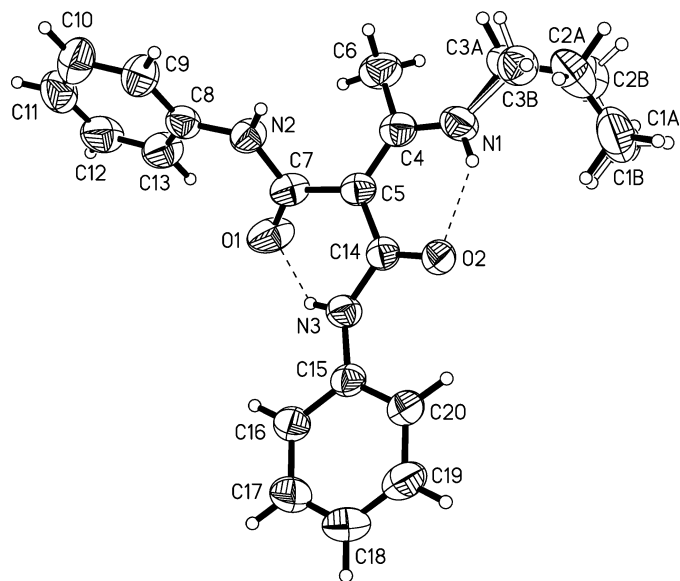
Figure 2
Diagram of polymorph (**II**) showing the atom-labelling scheme. Atomic displacement parameters are at the 50% probability level.

Table 4
Hydrogen-bond geometry (Å, °) for (**I**).

$Cg2$ is the centroid of the C15–C20 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$N\cdots$O2	0.90 (2)	1.87 (2)	2.623 (2)	139 (2)
N3—H3$N\cdots$O1	0.89 (2)	1.92 (2)	2.687 (2)	142.9 (19)
C6—H6$B\cdots$N2	0.98	2.45	2.943 (3)	111
C13—H13$\cdots$O1	0.95	2.37	2.905 (2)	115
C20—H20$\cdots$O2	0.95	2.29	2.854 (2)	117
N2—H2$N\cdots$O2^i	0.87 (2)	2.02 (2)	2.843 (2)	158 (2)
C10—H10$\cdots$O1^{ii}	0.95	2.76	3.635 (2)	154
C13—H13$\cdots Cg2^{iii}$	0.95	3.40	4.011 (2)	124

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

Table 5
Hydrogen-bond geometry (Å, °) for (**II**).

$Cg2$ is the centroid of the C15–C20 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$N\cdots$O2	0.91 (2)	1.92 (2)	2.638 (2)	135 (2)
N3—H3$N\cdots$O1	0.90 (3)	1.94 (3)	2.712 (2)	144 (2)
C6—H6$B\cdots$N2	0.98	2.46	2.968 (3)	112
C13—H13$\cdots$O1	0.95	2.33	2.879 (3)	116
C20—H20$\cdots$O2	0.95	2.30	2.887 (3)	119
N2—H2$N\cdots$O2^i	0.88 (2)	2.08 (2)	2.914 (2)	157 (2)
C9—H9$\cdots$O2^i	0.95	2.91	3.622 (3)	133
C13—H13$\cdots Cg2^{ii}$	0.95	3.37	3.960 (3)	122

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

by a weak C10—H10$\cdots$O1 interaction, resulting in a chain along the crystallographic *a*-axis direction in (**I**) (Fig. 4). In (**II**), these dimers are connected not *via* this C—H$\cdots$O contact, but by weak C—H$\cdots\pi$ interactions, forming intermolecular chains along the *c*-axis direction (Fig. 5). The latter are also observed in (**I**).

4. Database survey

Related structures are 2,2′-[benzylidenemethylenebis-(carbonylamino)]dibenzoic acid (Taga *et al.*, 1985), bis(*N,N*-diphenyl)(*m*-chlorobenzylidene)malonyldiamide (Kerr *et al.*, 1985; CSD refode: FACDES) and 1,1-bis(*N*-phenylcarbamoyl)-2-(*p*-chlorophenyl)ethylene (Kerr & Ashmore, 1973; CSD refode: PCMETY). Furthermore, several related push–pull
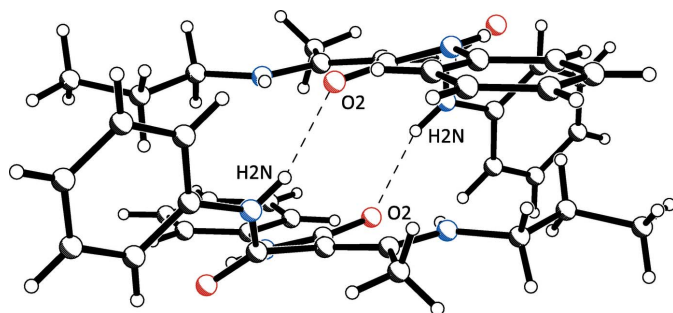
Figure 3
Intermolecular N—H$\cdots$O interactions leading to dimers in the crystal structure of (**I**), representative of both polymorphs.
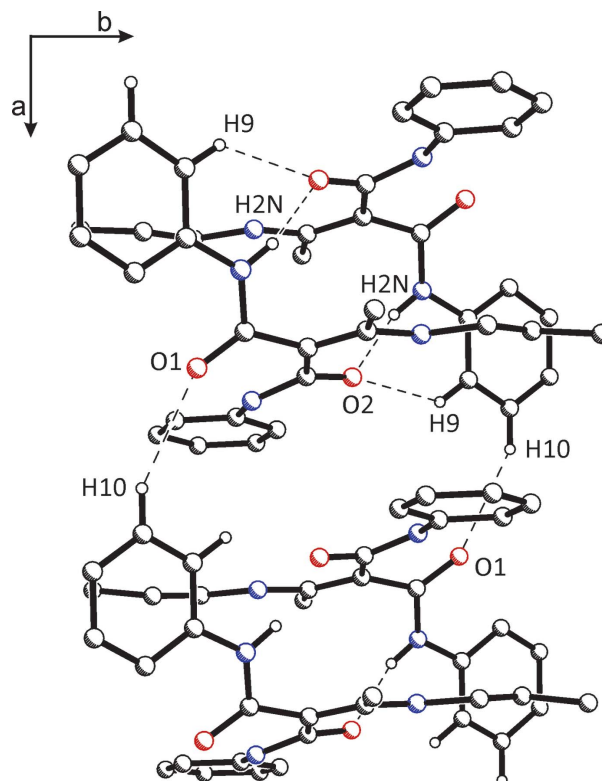
Figure 4
Packing diagram of polymorph (**I**) viewed along the *c* axis. Intermolecular N—H$\cdots$O and C—H$\cdots$O interactions are shown.

alkenes from cyclic ketene-*N,N*′-acetals have been prepared and structurally characterized (Ye *et al.*, 2010). Therein, the push–pull effect reduces the double-bond order by intramolecular charge transfer. This makes such alkenes interesting as substrates for second order non-linear optical materials.

5. Synthesis and crystallization

N,N′-Diphenyl-2-[1-(propylamino)ethylidene]propanediamide was obtained from the reaction of a silylated enamine (*N*-propyl-*N*-trimethylsilylprop-1-en-2-amine) and phenyl isocyanate. As shown in Fig. 6, insertion of Ph-NCO into both C—H bonds of the enamine takes place. This reaction is
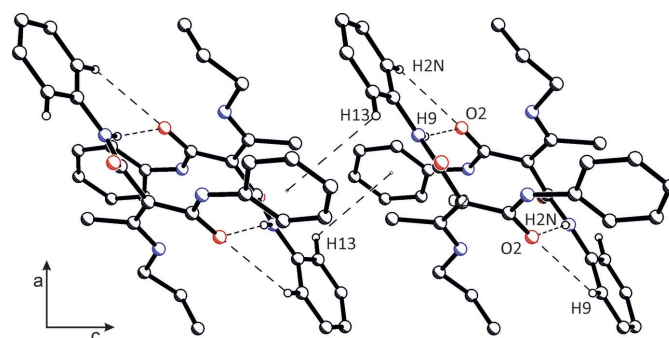
Figure 5
Packing diagram of polymorph (**II**) viewed along the *b* axis. Intermolecular N—H$\cdots$O, C—H$\cdots$O and C—H$\cdots\pi$ interactions are shown.

Table 6
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{20}H_{23}N_3O_2$	$C_{20}H_{23}N_3O_2$
M_r	337.41	337.41
Crystal system, space group	Monoclinic, $P2_1/n$	Tetragonal, $I4_1/a$
Temperature (K)	193	193
a, b, c (Å)	8.3881 (4), 24.3653 (9), 9.2614 (5)	27.7071 (11), 27.7071 (11), 9.4575 (4)
α, β, γ (°)	90, 107.724 (4), 90	90, 90, 90
V (Å^3)	1802.99 (15)	7260.4 (7)
Z	4	16
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.08	0.08
Crystal size (mm)	$0.48 \times 0.21 \times 0.18$	$0.49 \times 0.35 \times 0.25$
Data collection		
Diffractometer	Stoe IPDS 2	Stoe IPDS 2T
Absorption correction	Integration (*X-RED*; Stoe, 2009)	Integration (*X-RED*; Stoe, 2009)
T_{min}, T_{max}	0.820, 0.980	0.844, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18377, 3882, 2967	23893, 3884, 2635
R_{int}	0.054	0.042
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.639	0.637
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.129, 1.15	0.052, 0.132, 1.07
No. of reflections	3882	3884
No. of parameters	240	269
No. of restraints	0	69
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.14, −0.23	0.25, −0.19

Computer programs: *X-AREA* and *X-RED* (Stoe, 2009), *SHELXT* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b) and *ORTEP-3 for Windows* (Farrugia, 2012).

possible due to the lability of the β-hydrogen atoms of the enamine (Ozaki, 1972). Traces of water lead to the cleavage of the Si—N bond from the intermediate to yield the title compound.

To a solution of 0.46 g (3 mmol) *N*-propyl-*N*-trimethylsilylprop-1-en-2-amine in 10 mL of *n*-pentane was added
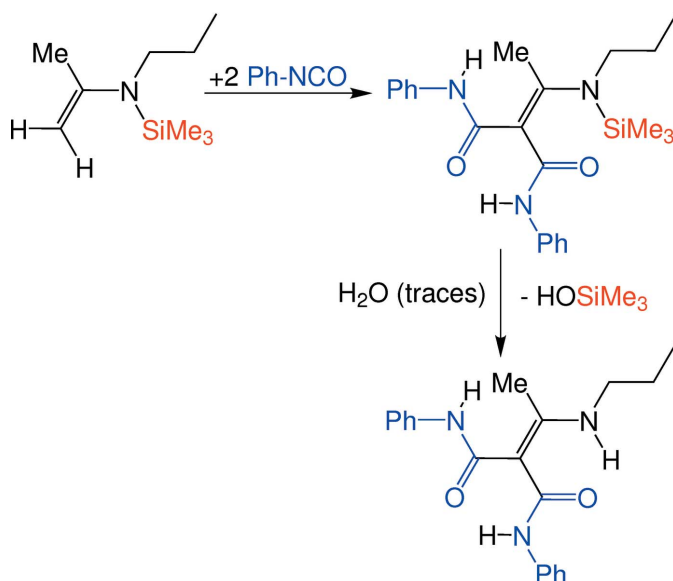
Figure 6
Reaction scheme for the synthesis of the title compounds.

dropwise 0.60 g (5 mmol) of phenylisocyanate at 273 K. After standing three days at room temperature, some crystals suitable for single-crystal X-ray diffraction were obtained. The polymorphs were recognised by their different crystal shapes: (I) forms small prisms, (II) forms large flat prisms. Both are colourless.

NMR spectroscopy showed that the batch product is a mixture of many components. Further purification of the product mixture was not successful.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 6. Hydrogen atoms bonded to C were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å for H(Ph), 0.99 for CH$_2$, and 0.98 Å for CH$_3$. U_{iso}(H) = xU_{eq}(C), where x = 1.2 for H(Ph) and CH$_2$, and 1.5 for CH$_3$. Hydrogen atoms on nitrogen were localized from residual electron-density maps and were freely refined.

Acknowledgements

research communications

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supporting information

Two polymorphs of *N,N′*-diphenyl-2-[1-(propylamino)ethylidene]propanediamide

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Computing details

For both structures, data collection: *X-AREA* (Stoe, 2009); cell refinement: *X-AREA* (Stoe, 2009); data reduction: *X-RED* (Stoe, 2009); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL2018* (Sheldrick, 2015b).

N,N′-Diphenyl-2-[1-(propylamino)ethylidene]propanediamide (I)

Crystal data

$C_{20}H_{23}N_3O_2$	$F(000) = 720$
$M_r = 337.41$	$D_x = 1.243$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.3881$ (4) Å	Cell parameters from 18377 reflections
$b = 24.3653$ (9) Å	$\theta = 2.3–27.4°$
$c = 9.2614$ (5) Å	$\mu = 0.08$ mm^{-1}
$\beta = 107.724$ (4)°	$T = 193$ K
$V = 1802.99$ (15) Å^3	Prism, colourless
$Z = 4$	$0.48 \times 0.21 \times 0.18$ mm

Data collection

Stoe IPDS 2 diffractometer	18377 measured reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	3882 independent reflections
	2967 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.054$
rotation method scans	$\theta_{max} = 27.0°$, $\theta_{min} = 2.5°$
Absorption correction: integration (X-RED; Stoe, 2009)	$h = -10 \rightarrow 10$
	$k = -30 \rightarrow 31$
$T_{min} = 0.820$, $T_{max} = 0.980$	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: mixed
$wR(F^2) = 0.129$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.15$	
3882 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.6249P]$
240 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.14$ e Å^{-3}

$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1490 (3)	1.22813 (9)	0.6450 (3)	0.0565 (6)
H1A	0.059051	1.234402	0.690216	0.085*
H1B	0.138400	1.254351	0.562369	0.085*
H1C	0.257591	1.233135	0.722392	0.085*
C2	0.1367 (3)	1.17012 (8)	0.5832 (2)	0.0457 (5)
H2A	0.034581	1.166745	0.495147	0.055*
H2B	0.234587	1.162517	0.547866	0.055*
C3	0.1304 (2)	1.12830 (7)	0.7020 (2)	0.0363 (4)
H3A	0.220902	1.135805	0.797292	0.044*
H3B	0.021949	1.131048	0.723328	0.044*
N1	0.15026 (19)	1.07318 (6)	0.64863 (18)	0.0342 (3)
H1N	0.187 (3)	1.0698 (10)	0.567 (3)	0.050 (6)*
C4	0.1460 (2)	1.02613 (7)	0.72048 (19)	0.0311 (4)
C5	0.1863 (2)	0.97588 (7)	0.66711 (19)	0.0297 (4)
C6	0.1047 (2)	1.03163 (8)	0.8671 (2)	0.0399 (4)
H6A	0.175144	1.060165	0.929658	0.060*
H6B	0.125317	0.996585	0.921533	0.060*
H6C	−0.013406	1.041718	0.845375	0.060*
C7	0.1491 (2)	0.92312 (7)	0.72906 (19)	0.0311 (4)
O1	0.24257 (16)	0.88268 (6)	0.75027 (15)	0.0413 (3)
N2	−0.00388 (19)	0.92087 (6)	0.75185 (18)	0.0336 (3)
H2N	−0.073 (3)	0.9468 (10)	0.708 (3)	0.049 (6)*
C8	−0.0758 (2)	0.87725 (7)	0.81029 (19)	0.0311 (4)
C9	−0.2493 (2)	0.87627 (8)	0.7747 (2)	0.0362 (4)
H9	−0.314313	0.903796	0.710646	0.043*
C10	−0.3278 (2)	0.83562 (8)	0.8319 (2)	0.0416 (4)
H10	−0.446393	0.835127	0.806474	0.050*
C11	−0.2340 (3)	0.79569 (8)	0.9259 (2)	0.0448 (5)
H11	−0.287648	0.767829	0.965915	0.054*
C12	−0.0622 (3)	0.79650 (9)	0.9612 (2)	0.0452 (5)
H12	0.002335	0.769047	1.025872	0.054*
C13	0.0176 (2)	0.83696 (8)	0.9033 (2)	0.0390 (4)
H13	0.136133	0.836958	0.927613	0.047*
C14	0.25399 (19)	0.97405 (7)	0.53946 (19)	0.0299 (4)
O2	0.25269 (15)	1.01470 (5)	0.45613 (14)	0.0342 (3)
N3	0.3185 (2)	0.92538 (7)	0.51188 (18)	0.0359 (4)
H3N	0.313 (3)	0.8986 (9)	0.576 (2)	0.041 (6)*
C15	0.3593 (2)	0.90910 (8)	0.3819 (2)	0.0333 (4)

C16	0.3682 (2)	0.85294 (9)	0.3598 (2)	0.0425 (5)
H16	0.347921	0.828183	0.431518	0.051*
C17	0.4061 (3)	0.83256 (10)	0.2347 (2)	0.0498 (5)
H17	0.412200	0.794052	0.221270	0.060*
C18	0.4352 (2)	0.86814 (10)	0.1293 (2)	0.0485 (5)
H18	0.459997	0.854333	0.042642	0.058*
C19	0.4277 (2)	0.92404 (10)	0.1514 (2)	0.0465 (5)
H19	0.447291	0.948603	0.078995	0.056*
C20	0.3919 (2)	0.94502 (8)	0.2779 (2)	0.0395 (4)
H20	0.389836	0.983552	0.292900	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0671 (15)	0.0358 (11)	0.0656 (15)	0.0032 (10)	0.0187 (12)	0.0015 (10)
C2	0.0514 (12)	0.0372 (11)	0.0476 (11)	0.0013 (9)	0.0140 (9)	−0.0014 (9)
C3	0.0352 (9)	0.0313 (9)	0.0425 (10)	0.0012 (7)	0.0122 (8)	−0.0075 (8)
N1	0.0357 (8)	0.0317 (8)	0.0375 (8)	0.0006 (6)	0.0142 (7)	−0.0033 (6)
C4	0.0251 (8)	0.0352 (9)	0.0332 (9)	−0.0010 (7)	0.0094 (7)	−0.0017 (7)
C5	0.0267 (8)	0.0323 (9)	0.0310 (8)	0.0009 (6)	0.0103 (7)	0.0006 (7)
C6	0.0433 (10)	0.0433 (11)	0.0375 (10)	0.0001 (8)	0.0186 (8)	−0.0047 (8)
C7	0.0289 (8)	0.0357 (9)	0.0298 (8)	0.0020 (7)	0.0106 (7)	0.0011 (7)
O1	0.0395 (7)	0.0422 (8)	0.0472 (8)	0.0115 (6)	0.0210 (6)	0.0118 (6)
N2	0.0292 (7)	0.0316 (8)	0.0418 (8)	0.0020 (6)	0.0137 (6)	0.0064 (7)
C8	0.0342 (9)	0.0313 (9)	0.0304 (8)	−0.0012 (7)	0.0137 (7)	−0.0011 (7)
C9	0.0334 (9)	0.0385 (10)	0.0389 (10)	0.0008 (7)	0.0143 (8)	0.0017 (8)
C10	0.0353 (10)	0.0450 (11)	0.0485 (11)	−0.0043 (8)	0.0186 (8)	−0.0006 (9)
C11	0.0471 (11)	0.0396 (11)	0.0529 (12)	−0.0077 (9)	0.0228 (9)	0.0053 (9)
C12	0.0451 (11)	0.0403 (11)	0.0505 (12)	0.0015 (8)	0.0150 (9)	0.0117 (9)
C13	0.0329 (9)	0.0402 (10)	0.0432 (10)	−0.0001 (8)	0.0106 (8)	0.0070 (8)
C14	0.0233 (7)	0.0337 (9)	0.0326 (9)	0.0006 (6)	0.0080 (6)	0.0011 (7)
O2	0.0344 (6)	0.0347 (7)	0.0373 (7)	0.0029 (5)	0.0165 (5)	0.0046 (5)
N3	0.0414 (8)	0.0329 (8)	0.0393 (8)	0.0073 (7)	0.0210 (7)	0.0036 (7)
C15	0.0255 (8)	0.0406 (10)	0.0352 (9)	0.0045 (7)	0.0115 (7)	−0.0016 (7)
C16	0.0421 (10)	0.0425 (11)	0.0459 (11)	0.0077 (8)	0.0180 (9)	−0.0017 (9)
C17	0.0481 (12)	0.0524 (13)	0.0495 (12)	0.0083 (9)	0.0158 (9)	−0.0144 (10)
C18	0.0359 (10)	0.0712 (15)	0.0390 (10)	0.0057 (10)	0.0124 (8)	−0.0138 (10)
C19	0.0372 (10)	0.0668 (14)	0.0397 (11)	0.0019 (9)	0.0181 (8)	0.0006 (10)
C20	0.0354 (10)	0.0450 (11)	0.0431 (10)	0.0026 (8)	0.0193 (8)	−0.0001 (8)

Geometric parameters (Å, º)

C1—C2	1.517 (3)	C9—C10	1.381 (3)
C1—H1A	0.9800	C9—H9	0.9500
C1—H1B	0.9800	C10—C11	1.381 (3)
C1—H1C	0.9800	C10—H10	0.9500
C2—C3	1.512 (3)	C11—C12	1.377 (3)
C2—H2A	0.9900	C11—H11	0.9500

C2—H2B	0.9900	C12—C13	1.388 (3)
C3—N1	1.458 (2)	C12—H12	0.9500
C3—H3A	0.9900	C13—H13	0.9500
C3—H3B	0.9900	C14—O2	1.254 (2)
N1—C4	1.331 (2)	C14—N3	1.360 (2)
N1—H1N	0.90 (2)	N3—C15	1.405 (2)
C4—C5	1.400 (2)	N3—H3N	0.89 (2)
C4—C6	1.506 (2)	C15—C20	1.389 (3)
C5—C14	1.460 (2)	C15—C16	1.389 (3)
C5—C7	1.479 (2)	C16—C17	1.384 (3)
C6—H6A	0.9800	C16—H16	0.9500
C6—H6B	0.9800	C17—C18	1.381 (3)
C6—H6C	0.9800	C17—H17	0.9500
C7—O1	1.237 (2)	C18—C19	1.382 (3)
C7—N2	1.364 (2)	C18—H18	0.9500
N2—C8	1.409 (2)	C19—C20	1.392 (3)
N2—H2N	0.87 (2)	C19—H19	0.9500
C8—C13	1.382 (3)	C20—H20	0.9500
C8—C9	1.391 (2)		
C2—C1—H1A	109.5	C9—C8—N2	117.48 (16)
C2—C1—H1B	109.5	C10—C9—C8	120.55 (18)
H1A—C1—H1B	109.5	C10—C9—H9	119.7
C2—C1—H1C	109.5	C8—C9—H9	119.7
H1A—C1—H1C	109.5	C11—C10—C9	120.02 (18)
H1B—C1—H1C	109.5	C11—C10—H10	120.0
C3—C2—C1	111.53 (18)	C9—C10—H10	120.0
C3—C2—H2A	109.3	C12—C11—C10	119.58 (18)
C1—C2—H2A	109.3	C12—C11—H11	120.2
C3—C2—H2B	109.3	C10—C11—H11	120.2
C1—C2—H2B	109.3	C11—C12—C13	120.78 (19)
H2A—C2—H2B	108.0	C11—C12—H12	119.6
N1—C3—C2	109.93 (15)	C13—C12—H12	119.6
N1—C3—H3A	109.7	C8—C13—C12	119.77 (18)
C2—C3—H3A	109.7	C8—C13—H13	120.1
N1—C3—H3B	109.7	C12—C13—H13	120.1
C2—C3—H3B	109.7	O2—C14—N3	120.18 (15)
H3A—C3—H3B	108.2	O2—C14—C5	122.81 (16)
C4—N1—C3	126.89 (16)	N3—C14—C5	117.00 (15)
C4—N1—H1N	114.0 (15)	C14—N3—C15	128.45 (16)
C3—N1—H1N	118.2 (15)	C14—N3—H3N	114.1 (14)
N1—C4—C5	122.05 (16)	C15—N3—H3N	116.0 (14)
N1—C4—C6	114.99 (16)	C20—C15—C16	119.20 (17)
C5—C4—C6	122.87 (16)	C20—C15—N3	124.55 (17)
C4—C5—C14	120.53 (15)	C16—C15—N3	116.25 (17)
C4—C5—C7	121.41 (15)	C17—C16—C15	120.9 (2)
C14—C5—C7	117.88 (15)	C17—C16—H16	119.6
C4—C6—H6A	109.5	C15—C16—H16	119.6

C4—C6—H6B	109.5	C18—C17—C16	120.1 (2)
H6A—C6—H6B	109.5	C18—C17—H17	119.9
C4—C6—H6C	109.5	C16—C17—H17	119.9
H6A—C6—H6C	109.5	C17—C18—C19	119.21 (19)
H6B—C6—H6C	109.5	C17—C18—H18	120.4
O1—C7—N2	121.60 (16)	C19—C18—H18	120.4
O1—C7—C5	123.75 (15)	C18—C19—C20	121.2 (2)
N2—C7—C5	114.50 (15)	C18—C19—H19	119.4
C7—N2—C8	128.54 (16)	C20—C19—H19	119.4
C7—N2—H2N	115.0 (15)	C15—C20—C19	119.38 (19)
C8—N2—H2N	115.2 (15)	C15—C20—H20	120.3
C13—C8—C9	119.29 (17)	C19—C20—H20	120.3
C13—C8—N2	123.20 (16)		

C1—C2—C3—N1	−169.39 (17)	C10—C11—C12—C13	0.0 (3)
C2—C3—N1—C4	−177.75 (17)	C9—C8—C13—C12	−0.6 (3)
C3—N1—C4—C5	−172.23 (16)	N2—C8—C13—C12	177.48 (18)
C3—N1—C4—C6	4.4 (3)	C11—C12—C13—C8	0.6 (3)
N1—C4—C5—C14	7.3 (3)	C4—C5—C14—O2	−12.5 (3)
C6—C4—C5—C14	−169.03 (16)	C7—C5—C14—O2	162.54 (15)
N1—C4—C5—C7	−167.58 (16)	C4—C5—C14—N3	168.22 (15)
C6—C4—C5—C7	16.1 (2)	C7—C5—C14—N3	−16.7 (2)
C4—C5—C7—O1	−142.19 (18)	O2—C14—N3—C15	−13.5 (3)
C14—C5—C7—O1	42.8 (2)	C5—C14—N3—C15	165.78 (17)
C4—C5—C7—N2	42.2 (2)	C14—N3—C15—C20	22.0 (3)
C14—C5—C7—N2	−132.82 (16)	C14—N3—C15—C16	−158.64 (18)
O1—C7—N2—C8	5.0 (3)	C20—C15—C16—C17	−1.1 (3)
C5—C7—N2—C8	−179.29 (16)	N3—C15—C16—C17	179.48 (18)
C7—N2—C8—C13	24.0 (3)	C15—C16—C17—C18	−0.3 (3)
C7—N2—C8—C9	−157.83 (18)	C16—C17—C18—C19	0.7 (3)
C13—C8—C9—C10	0.1 (3)	C17—C18—C19—C20	0.2 (3)
N2—C8—C9—C10	−178.08 (17)	C16—C15—C20—C19	2.0 (3)
C8—C9—C10—C11	0.4 (3)	N3—C15—C20—C19	−178.67 (17)
C9—C10—C11—C12	−0.5 (3)	C18—C19—C20—C15	−1.5 (3)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C15–C20 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2	0.90 (2)	1.87 (2)	2.623 (2)	139 (2)
N3—H3*N*···O1	0.89 (2)	1.92 (2)	2.687 (2)	142.9 (19)
C6—H6*B*···N2	0.98	2.45	2.943 (3)	111
C13—H13···O1	0.95	2.37	2.905 (2)	115
C20—H20···O2	0.95	2.29	2.854 (2)	117
N2—H2*N*···O2i	0.87 (2)	2.02 (2)	2.843 (2)	158 (2)

C10—H10···O1^{ii}	0.95	2.76	3.635 (2)	154
C13—H13···$Cg2^{iii}$	0.95	3.40	4.011 (2)	124

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

N,N'-Diphenyl-2-[1-(propylamino)ethylidene]propanediamide (II)

Crystal data

$C_{20}H_{23}N_3O_2$	$D_x = 1.235$ Mg m^{-3}
$M_r = 337.41$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Tetragonal, $I4_1/a$	Cell parameters from 23893 reflections
$a = 27.7071$ (11) Å	$\theta = 2.7$–27.2°
$c = 9.4575$ (4) Å	$\mu = 0.08$ mm^{-1}
$V = 7260.4$ (7) Å^3	$T = 193$ K
$Z = 16$	Prism, colourless
$F(000) = 2880$	$0.49 \times 0.35 \times 0.25$ mm

Data collection

Stoe IPDS 2T diffractometer	23893 measured reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	3884 independent reflections
	2635 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.042$
rotation method scans	$\theta_{max} = 26.9°$, $\theta_{min} = 2.7°$
Absorption correction: integration (X-RED; Stoe, 2009)	$h = -34 \rightarrow 30$
	$k = -34 \rightarrow 35$
$T_{min} = 0.844$, $T_{max} = 0.980$	$l = -12 \rightarrow 11$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.052$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.132$	
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 6.4556P]$ where $P = (F_o^2 + 2F_c^2)/3$
3884 reflections	
269 parameters	$(\Delta/\sigma)_{max} = 0.001$
69 restraints	$\Delta\rho_{max} = 0.25$ e Å^{-3}
	$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
C1A	0.33034 (19)	0.4509 (2)	1.0073 (5)	0.1009 (15)	0.794 (7)
H1A	0.345612	0.480495	1.042488	0.151*	0.794 (7)
H1B	0.315992	0.433244	1.086538	0.151*	0.794 (7)
H1C	0.305092	0.459356	0.939020	0.151*	0.794 (7)
C2A	0.36613 (16)	0.42112 (13)	0.9393 (4)	0.0792 (12)	0.794 (7)

H2A	0.349729	0.392523	0.898911	0.095*	0.794 (7)
H2B	0.388915	0.409434	1.012267	0.095*	0.794 (7)
C3A	0.39475 (11)	0.44513 (12)	0.8236 (4)	0.0557 (9)	0.794 (7)
H3A	0.416173	0.421327	0.777213	0.067*	0.794 (7)
H3B	0.372703	0.458651	0.751383	0.067*	0.794 (7)
C1B	0.3142 (5)	0.4689 (5)	0.9652 (16)	0.064 (4)	0.206 (7)
H1D	0.335316	0.489802	1.021394	0.095*	0.206 (7)
H1E	0.294887	0.448625	1.028587	0.095*	0.206 (7)
H1F	0.292641	0.488873	0.907398	0.095*	0.206 (7)
C2B	0.3429 (5)	0.4388 (5)	0.8749 (18)	0.082 (4)	0.206 (7)
H2C	0.334739	0.448684	0.777208	0.098*	0.206 (7)
H2D	0.329972	0.405792	0.886790	0.098*	0.206 (7)
C3B	0.3960 (4)	0.4337 (4)	0.8773 (17)	0.060 (4)	0.206 (7)
H3C	0.406400	0.416664	0.790496	0.072*	0.206 (7)
H3D	0.405204	0.413461	0.959305	0.072*	0.206 (7)
N1	0.42335 (7)	0.48356 (7)	0.8871 (2)	0.0554 (5)	
H1N	0.4203 (8)	0.4899 (8)	0.981 (3)	0.062 (7)*	
C4	0.45371 (7)	0.51141 (7)	0.8148 (2)	0.0489 (5)	
C5	0.47728 (7)	0.55038 (7)	0.8774 (2)	0.0441 (4)	
C6	0.45777 (9)	0.50023 (10)	0.6592 (2)	0.0673 (6)	
H6A	0.474937	0.469611	0.646512	0.101*	
H6B	0.475621	0.526138	0.611807	0.101*	
H6C	0.425402	0.497686	0.618089	0.101*	
C7	0.51595 (8)	0.57654 (7)	0.8002 (2)	0.0503 (5)	
O1	0.51926 (7)	0.62093 (5)	0.79818 (17)	0.0724 (5)	
N2	0.54997 (6)	0.54761 (6)	0.73837 (19)	0.0496 (4)	
H2N	0.5496 (8)	0.5170 (8)	0.764 (2)	0.055 (6)*	
C8	0.59020 (8)	0.56177 (7)	0.6563 (2)	0.0486 (5)	
C9	0.62718 (8)	0.52880 (9)	0.6397 (2)	0.0607 (6)	
H9	0.625036	0.497964	0.683170	0.073*	
C10	0.66752 (9)	0.54064 (11)	0.5594 (3)	0.0747 (7)	
H10	0.692931	0.517901	0.548843	0.090*	
C11	0.67088 (10)	0.58508 (11)	0.4952 (3)	0.0752 (7)	
H11	0.698696	0.593338	0.441738	0.090*	
C12	0.63374 (11)	0.61724 (9)	0.5093 (3)	0.0758 (8)	
H12	0.635694	0.647678	0.463431	0.091*	
C13	0.59336 (10)	0.60625 (8)	0.5892 (3)	0.0660 (6)	
H13	0.567914	0.629032	0.598067	0.079*	
C14	0.46565 (7)	0.56580 (6)	1.0214 (2)	0.0409 (4)	
O2	0.43901 (5)	0.54185 (4)	1.10290 (14)	0.0463 (3)	
N3	0.48566 (6)	0.60834 (6)	1.06502 (18)	0.0480 (4)	
H3N	0.5014 (9)	0.6240 (9)	0.996 (3)	0.069 (7)*	
C15	0.48675 (7)	0.62908 (7)	1.2011 (2)	0.0441 (4)	
C16	0.51880 (8)	0.66737 (7)	1.2202 (2)	0.0539 (5)	
H16	0.538506	0.677647	1.143708	0.065*	
C17	0.52215 (9)	0.69048 (8)	1.3491 (3)	0.0652 (6)	
H17	0.543793	0.716791	1.360352	0.078*	
C18	0.49444 (10)	0.67569 (9)	1.4611 (3)	0.0726 (7)	

H18	0.496925	0.691430	1.550003	0.087*
C19	0.46305 (10)	0.63785 (9)	1.4430 (3)	0.0714 (7)
H19	0.443956	0.627485	1.520741	0.086*
C20	0.45852 (8)	0.61441 (8)	1.3144 (2)	0.0556 (5)
H20	0.436309	0.588537	1.303791	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.092 (3)	0.118 (3)	0.093 (3)	−0.055 (2)	0.009 (2)	−0.002 (2)
C2A	0.0903 (19)	0.0684 (16)	0.0790 (18)	−0.0305 (14)	−0.0128 (15)	0.0055 (13)
C3A	0.0578 (14)	0.0513 (14)	0.0580 (15)	−0.0049 (11)	−0.0094 (12)	−0.0071 (12)
C1B	0.060 (4)	0.060 (5)	0.071 (5)	−0.001 (3)	0.005 (3)	0.003 (3)
C2B	0.081 (5)	0.082 (5)	0.084 (5)	−0.001 (2)	0.000 (2)	−0.004 (2)
C3B	0.060 (4)	0.061 (4)	0.059 (4)	−0.001 (2)	−0.002 (2)	−0.002 (2)
N1	0.0518 (10)	0.0524 (10)	0.0620 (12)	−0.0028 (8)	−0.0085 (9)	−0.0123 (9)
C4	0.0460 (11)	0.0499 (11)	0.0508 (11)	0.0097 (9)	−0.0066 (9)	−0.0037 (9)
C5	0.0471 (11)	0.0411 (10)	0.0440 (10)	0.0058 (8)	−0.0026 (9)	0.0001 (8)
C6	0.0674 (15)	0.0805 (16)	0.0539 (13)	0.0079 (12)	−0.0086 (11)	−0.0185 (12)
C7	0.0650 (13)	0.0431 (11)	0.0428 (10)	0.0069 (9)	0.0047 (10)	0.0027 (9)
O1	0.1109 (14)	0.0413 (8)	0.0649 (10)	0.0050 (8)	0.0316 (10)	0.0050 (7)
N2	0.0557 (10)	0.0402 (9)	0.0528 (10)	0.0032 (7)	0.0092 (8)	0.0039 (8)
C8	0.0553 (12)	0.0474 (11)	0.0432 (10)	−0.0078 (9)	0.0026 (9)	−0.0018 (9)
C9	0.0566 (13)	0.0656 (14)	0.0598 (13)	0.0030 (11)	0.0044 (11)	0.0078 (11)
C10	0.0574 (14)	0.094 (2)	0.0726 (16)	0.0023 (13)	0.0121 (13)	0.0023 (15)
C11	0.0698 (17)	0.0887 (19)	0.0671 (15)	−0.0283 (15)	0.0151 (13)	−0.0060 (14)
C12	0.100 (2)	0.0582 (14)	0.0691 (16)	−0.0249 (14)	0.0257 (15)	−0.0036 (12)
C13	0.0837 (17)	0.0497 (12)	0.0646 (14)	−0.0042 (11)	0.0186 (13)	0.0022 (11)
C14	0.0398 (10)	0.0369 (9)	0.0459 (10)	0.0048 (7)	−0.0006 (8)	0.0017 (8)
O2	0.0458 (7)	0.0411 (7)	0.0521 (8)	−0.0017 (6)	0.0064 (6)	−0.0013 (6)
N3	0.0581 (10)	0.0397 (9)	0.0462 (9)	−0.0063 (7)	0.0079 (8)	−0.0011 (7)
C15	0.0453 (10)	0.0369 (10)	0.0501 (11)	0.0060 (8)	0.0033 (9)	−0.0027 (8)
C16	0.0558 (12)	0.0415 (11)	0.0645 (13)	−0.0025 (9)	0.0075 (10)	−0.0076 (10)
C17	0.0664 (15)	0.0504 (12)	0.0789 (16)	−0.0022 (11)	0.0022 (13)	−0.0192 (12)
C18	0.0843 (18)	0.0642 (15)	0.0694 (16)	0.0026 (13)	0.0052 (14)	−0.0263 (13)
C19	0.0795 (17)	0.0749 (16)	0.0598 (14)	−0.0014 (13)	0.0221 (13)	−0.0151 (13)
C20	0.0565 (12)	0.0522 (12)	0.0580 (13)	−0.0043 (9)	0.0133 (10)	−0.0099 (10)

Geometric parameters (Å, º)

C1A—C2A	1.442 (6)	C7—N2	1.369 (3)
C1A—H1A	0.9800	N2—C8	1.414 (3)
C1A—H1B	0.9800	N2—H2N	0.88 (2)
C1A—H1C	0.9800	C8—C9	1.382 (3)
C2A—C3A	1.506 (5)	C8—C13	1.389 (3)
C2A—H2A	0.9900	C9—C10	1.390 (3)
C2A—H2B	0.9900	C9—H9	0.9500
C3A—N1	1.457 (3)	C10—C11	1.376 (4)

C3A—H3A	0.9900	C10—H10	0.9500
C3A—H3B	0.9900	C11—C12	1.368 (4)
C1B—C2B	1.435 (14)	C11—H11	0.9500
C1B—H1D	0.9800	C12—C13	1.384 (3)
C1B—H1E	0.9800	C12—H12	0.9500
C1B—H1F	0.9800	C13—H13	0.9500
C2B—C3B	1.477 (14)	C14—O2	1.257 (2)
C2B—H2C	0.9900	C14—N3	1.366 (2)
C2B—H2D	0.9900	N3—C15	1.410 (3)
C3B—N1	1.580 (12)	N3—H3N	0.90 (3)
C3B—H3C	0.9900	C15—C20	1.387 (3)
C3B—H3D	0.9900	C15—C16	1.395 (3)
N1—C4	1.331 (3)	C16—C17	1.380 (3)
N1—H1N	0.91 (2)	C16—H16	0.9500
C4—C5	1.394 (3)	C17—C18	1.370 (4)
C4—C6	1.508 (3)	C17—H17	0.9500
C5—C14	1.463 (3)	C18—C19	1.373 (4)
C5—C7	1.485 (3)	C18—H18	0.9500
C6—H6A	0.9800	C19—C20	1.385 (3)
C6—H6B	0.9800	C19—H19	0.9500
C6—H6C	0.9800	C20—H20	0.9500
C7—O1	1.234 (2)		
C2A—C1A—H1A	109.5	H6A—C6—H6C	109.5
C2A—C1A—H1B	109.5	H6B—C6—H6C	109.5
H1A—C1A—H1B	109.5	O1—C7—N2	121.7 (2)
C2A—C1A—H1C	109.5	O1—C7—C5	123.24 (19)
H1A—C1A—H1C	109.5	N2—C7—C5	114.91 (17)
H1B—C1A—H1C	109.5	C7—N2—C8	127.97 (18)
C1A—C2A—C3A	115.7 (3)	C7—N2—H2N	115.9 (14)
C1A—C2A—H2A	108.4	C8—N2—H2N	115.3 (14)
C3A—C2A—H2A	108.4	C9—C8—C13	119.2 (2)
C1A—C2A—H2B	108.4	C9—C8—N2	117.63 (18)
C3A—C2A—H2B	108.4	C13—C8—N2	123.1 (2)
H2A—C2A—H2B	107.4	C8—C9—C10	120.2 (2)
N1—C3A—C2A	108.1 (3)	C8—C9—H9	119.9
N1—C3A—H3A	110.1	C10—C9—H9	119.9
C2A—C3A—H3A	110.1	C11—C10—C9	120.4 (3)
N1—C3A—H3B	110.1	C11—C10—H10	119.8
C2A—C3A—H3B	110.1	C9—C10—H10	119.8
H3A—C3A—H3B	108.4	C12—C11—C10	119.3 (2)
C2B—C1B—H1D	109.5	C12—C11—H11	120.4
C2B—C1B—H1E	109.5	C10—C11—H11	120.4
H1D—C1B—H1E	109.5	C11—C12—C13	121.2 (2)
C2B—C1B—H1F	109.5	C11—C12—H12	119.4
H1D—C1B—H1F	109.5	C13—C12—H12	119.4
H1E—C1B—H1F	109.5	C12—C13—C8	119.7 (2)
C1B—C2B—C3B	126.9 (13)	C12—C13—H13	120.1

C1B—C2B—H2C	105.6	C8—C13—H13	120.1
C3B—C2B—H2C	105.6	O2—C14—N3	120.55 (18)
C1B—C2B—H2D	105.6	O2—C14—C5	123.10 (17)
C3B—C2B—H2D	105.6	N3—C14—C5	116.35 (17)
H2C—C2B—H2D	106.1	C14—N3—C15	129.51 (17)
C2B—C3B—N1	113.2 (10)	C14—N3—H3N	113.2 (16)
C2B—C3B—H3C	108.9	C15—N3—H3N	117.2 (16)
N1—C3B—H3C	108.9	C20—C15—C16	118.78 (19)
C2B—C3B—H3D	108.9	C20—C15—N3	125.00 (18)
N1—C3B—H3D	108.9	C16—C15—N3	116.23 (18)
H3C—C3B—H3D	107.8	C17—C16—C15	120.7 (2)
C4—N1—C3A	123.8 (2)	C17—C16—H16	119.7
C4—N1—C3B	141.3 (6)	C15—C16—H16	119.7
C4—N1—H1N	116.8 (15)	C18—C17—C16	120.4 (2)
C3A—N1—H1N	119.5 (15)	C18—C17—H17	119.8
C3B—N1—H1N	100.4 (16)	C16—C17—H17	119.8
N1—C4—C5	121.78 (19)	C17—C18—C19	119.2 (2)
N1—C4—C6	115.5 (2)	C17—C18—H18	120.4
C5—C4—C6	122.6 (2)	C19—C18—H18	120.4
C4—C5—C14	121.24 (18)	C18—C19—C20	121.6 (2)
C4—C5—C7	120.47 (18)	C18—C19—H19	119.2
C14—C5—C7	118.27 (17)	C20—C19—H19	119.2
C4—C6—H6A	109.5	C19—C20—C15	119.3 (2)
C4—C6—H6B	109.5	C19—C20—H20	120.3
H6A—C6—H6B	109.5	C15—C20—H20	120.3
C4—C6—H6C	109.5		
C1A—C2A—C3A—N1	65.0 (4)	C8—C9—C10—C11	−0.4 (4)
C1B—C2B—C3B—N1	−46 (2)	C9—C10—C11—C12	−1.0 (4)
C2A—C3A—N1—C4	178.5 (3)	C10—C11—C12—C13	1.3 (4)
C2B—C3B—N1—C4	−116.6 (12)	C11—C12—C13—C8	−0.2 (4)
C3A—N1—C4—C5	174.5 (2)	C9—C8—C13—C12	−1.3 (4)
C3B—N1—C4—C5	−166.6 (8)	N2—C8—C13—C12	−179.3 (2)
C3A—N1—C4—C6	−1.1 (3)	C4—C5—C14—O2	9.5 (3)
C3B—N1—C4—C6	17.9 (9)	C7—C5—C14—O2	−168.94 (17)
N1—C4—C5—C14	−7.0 (3)	C4—C5—C14—N3	−170.85 (17)
C6—C4—C5—C14	168.25 (18)	C7—C5—C14—N3	10.7 (2)
N1—C4—C5—C7	171.42 (18)	O2—C14—N3—C15	9.3 (3)
C6—C4—C5—C7	−13.4 (3)	C5—C14—N3—C15	−170.35 (18)
C4—C5—C7—O1	136.4 (2)	C14—N3—C15—C20	−14.1 (3)
C14—C5—C7—O1	−45.1 (3)	C14—N3—C15—C16	166.21 (19)
C4—C5—C7—N2	−47.7 (3)	C20—C15—C16—C17	−0.4 (3)
C14—C5—C7—N2	130.73 (19)	N3—C15—C16—C17	179.2 (2)
O1—C7—N2—C8	−5.4 (3)	C15—C16—C17—C18	0.9 (4)
C5—C7—N2—C8	178.67 (19)	C16—C17—C18—C19	−0.5 (4)
C7—N2—C8—C9	161.2 (2)	C17—C18—C19—C20	−0.3 (4)
C7—N2—C8—C13	−20.8 (3)	C18—C19—C20—C15	0.7 (4)
C13—C8—C9—C10	1.6 (3)	C16—C15—C20—C19	−0.3 (3)

N2—C8—C9—C10	179.6 (2)	N3—C15—C20—C19	180.0 (2)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C15–C20 ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*N*⋯O2	0.91 (2)	1.92 (2)	2.638 (2)	135 (2)
N3—H3*N*⋯O1	0.90 (3)	1.94 (3)	2.712 (2)	144 (2)
C6—H6*B*⋯N2	0.98	2.46	2.968 (3)	112
C13—H13⋯O1	0.95	2.33	2.879 (3)	116
C20—H20⋯O2	0.95	2.30	2.887 (3)	119
N2—H2*N*⋯O2ⁱ	0.88 (2)	2.08 (2)	2.914 (2)	157 (2)
C9—H9⋯O2ⁱ	0.95	2.91	3.622 (3)	133
C13—H13⋯*Cg*2ⁱⁱ	0.95	3.37	3.960 (3)	122

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