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# *N*,*N*′-Diphenylsuberamide

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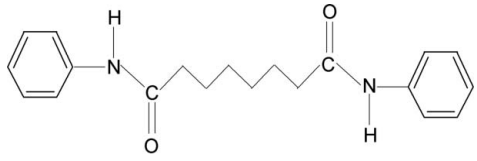
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.076; $wR$ factor = 0.203; data-to-parameter ratio = 13.5.

In the title compound (systematic name: *N*,*N*′-diphenyloctanediamide), $C_{20}H_{24}N_2O_2$, the two phenyl rings make an interplanar angle of 76.5 (2)°. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds, which link the molecules into chains running along the *b* axis. The crystal studied was non-merohedrally twinned, the fractional contribution of the minor twin component being 0.203 (2).

## Related literature

For related structures, see: Gowda *et al.* (2007, 2009*a*,*b*).



## Experimental

### *Crystal data*

$C_{20}H_{24}N_2O_2$
$M_r$ = 324.41
Monoclinic, $C2/c$
$a$ = 18.2267 (9) Å
$b$ = 5.03097 (15) Å
$c$ = 38.1436 (15) Å
$\beta$ = 96.517 (4)°
$V$ = 3475.1 (2) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 295 K
0.58 × 0.33 × 0.05 mm

### *Data collection*

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: analytical (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.957, $T_{max}$ = 0.996
27788 measured reflections
3027 independent reflections
2524 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.064

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.203
$S$ = 1.09
3027 reflections
224 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···O1$^{i}$ | 0.84 (3) | 2.17 (3) | 3.004 (4) | 173 (4) |
| N2—H2*N*···O2$^{ii}$ | 0.84 (3) | 2.13 (3) | 2.937 (4) | 161 (4) |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2009) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5267).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o1363 [ **doi:10.1107/S1600536810017344** ]

# *N*,*N*'-Diphenylsuberamide

**B. T. Gowda, M. Tokarcík, V. Z. Rodrigues, J. Kozísek and H. Fuess**

## Comment

The amide moiety is an important constituent of many biologically significant compounds. As a part of studying the effect of ring and side chain substitutions on the structures of this class of compounds (Gowda *et al.*, 2007; 2009*a,b*), the crystal structure of *N*,*N*-bis(phenyl)-suberamide has been determined (I) (Fig. 1).

In the structure, the two phenyl rings make an interplanar angle of 76.5 (2)°. The plane of the aliphatic group C2/C7 makes dihedral angles of 26.3 (5)° with the amide group (N1, H1N, C1, O1) and 27.2 (5)° with the amide group (N2, H2N, C8, O2). The conformations of the amide groups with respect to the attached phenyl rings are given by the torsion angles of C14—C9—N1—C1 = -38.0 (6)° and C16—C15—N2—C8 = -42.2 (6)°. The structure is stabilized by two intramolecular hydrogen bonds (Table 1). The intermolecular N–H···O hydrogen bonds link the molecules into the chains running along the *b*-axis of the crystal (Fig. 2). The crystal is merohedrally twinned with the twin fraction of 0.203 (2).

## Experimental

Suberic acid (0.3 mol) was heated with thionyl chloride (1.2 mol) at 120°C for 4 hours. The acid chloride obtained was treated with aniline (0.6 mol). The product obtained was added to crushed ice to obtain the white precipitate. It was thoroughly washed with water and then with saturated sodium bicarbonate solution and washed again with water. It was then given a wash with 2 N HCl. It was again washed with water, filtered, dried and recrystallised to constant point (186-188°C) from ethanol-Tetrahydrofuran mixture in the ratio 1:4.

Plate like colourless single crystals of the title compound used in X-ray diffraction studies were obtained by a slow evaporation of its solution at room temperature.

## Refinement

The crystal used for data collection was a non-merohedral twin. The twin law was found to be a twofold axis about the [1 0 4] direct lattice direction. The final refinement was made using the HKLF4 format of the HKL file, and using the INS file having the twin matrix (-1 0 0 / 0 -1 0 / 0.5 0 1) in the TWIN instruction. The fractional contribution of the minor twin component refined to 0.203 (2). The C-bounded hydrogen atoms were positioned with idealized geometry using a riding model with C–H = 0.93 Å or 0.97 Å. Amide H atoms were refined with N–H distance restrained to 0.85 (3) Å. The $U_{iso}$(H) values were set at 1.2$U_{eq}$(C, N).

## Figures

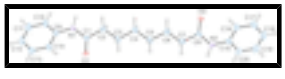

Fig. 1. Molecular structure of (I) showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radii.

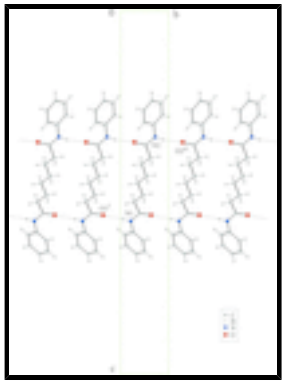

Fig. 2. Part of crystal structure of (I) viewed down the *a*-axis. Intermolecular N–H···O hydrogen bonds (shown as dashed lines) connect the molecules into chains running along the *b*-axis of the crystal. Symmetry codes (i): *x*, *y*-1, *z*; (ii): *x*, *y*+1, *z*.

## *N*,*N*'-Diphenyloctanediamide

### *Crystal data*

| | |
|---|---|
| $C_{20}H_{24}N_2O_2$ | $F(000) = 1392$ |
| $M_r = 324.41$ | $D_x = 1.24$ Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 7864 reflections |
| $a = 18.2267$ (9) Å | θ = 1.9–27.4° |
| $b = 5.03097$ (15) Å | μ = 0.08 mm$^{-1}$ |
| $c = 38.1436$ (15) Å | $T = 295$ K |
| β = 96.517 (4)° | Plate, colourless |
| $V = 3475.1$ (2) Å$^3$ | 0.58 × 0.33 × 0.05 mm |
| $Z = 8$ | |

### *Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini R CCD diffractometer | 3027 independent reflections |
| graphite | 2524 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.434 pixels mm$^{-1}$ | $R_{int} = 0.064$ |
| ω scans | $\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$ |
| Absorption correction: analytical (CrysAlis Pro; Oxford Diffraction, 2009) | $h = -21 \rightarrow 21$ |
| $T_{min} = 0.957$, $T_{max} = 0.996$ | $k = -5 \rightarrow 5$ |
| 27788 measured reflections | $l = -45 \rightarrow 45$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.076$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.203$ | H atoms treated by a mixture of independent and constrained refinement |

| | |
|---|---|
| $S$ = 1.09 | $w = 1/[\sigma^2(F_o^2) + (0.0865P)^2 + 8.373P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3027 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 224 parameters | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |
| 2 restraints | $\Delta\rho_{min} = -0.22$ 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.

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.0479 (2) | 0.3940 (7) | 0.55627 (10) | 0.0357 (9) |
| C2 | 0.0772 (2) | 0.2805 (8) | 0.52403 (10) | 0.0392 (9) |
| H2A | 0.0358 | 0.2378 | 0.5067 | 0.047* |
| H2B | 0.1029 | 0.1158 | 0.5306 | 0.047* |
| C3 | 0.1291 (2) | 0.4621 (8) | 0.50714 (10) | 0.0398 (9) |
| H3A | 0.1732 | 0.489 | 0.5235 | 0.048* |
| H3B | 0.1055 | 0.6337 | 0.5028 | 0.048* |
| C4 | 0.1511 (2) | 0.3560 (8) | 0.47276 (10) | 0.0398 (9) |
| H4A | 0.1068 | 0.3257 | 0.4567 | 0.048* |
| H4B | 0.1754 | 0.1857 | 0.4772 | 0.048* |
| C5 | 0.2020 (2) | 0.5373 (8) | 0.45507 (9) | 0.0415 (10) |
| H5A | 0.247 | 0.5627 | 0.4709 | 0.05* |
| H5B | 0.1784 | 0.7095 | 0.4514 | 0.05* |
| C6 | 0.2222 (2) | 0.4363 (8) | 0.42003 (10) | 0.0417 (10) |
| H6A | 0.2457 | 0.2638 | 0.4235 | 0.05* |
| H6B | 0.1775 | 0.4133 | 0.404 | 0.05* |
| C7 | 0.2735 (2) | 0.6215 (8) | 0.40346 (10) | 0.0416 (10) |
| H7A | 0.3186 | 0.6418 | 0.4194 | 0.05* |
| H7B | 0.2505 | 0.795 | 0.4004 | 0.05* |
| C8 | 0.2930 (2) | 0.5254 (7) | 0.36811 (10) | 0.0388 (9) |
| C9 | −0.0140 (2) | 0.2611 (7) | 0.60821 (9) | 0.0343 (8) |
| C10 | −0.0691 (2) | 0.0877 (9) | 0.61530 (10) | 0.0459 (10) |
| H10 | −0.0822 | −0.0522 | 0.5999 | 0.055* |
| C11 | −0.1051 (3) | 0.1199 (10) | 0.64514 (11) | 0.0565 (12) |
| H11 | −0.1425 | 0.0034 | 0.6497 | 0.068* |
| C12 | −0.0851 (3) | 0.3247 (10) | 0.66783 (11) | 0.0595 (13) |
| H12 | −0.109 | 0.3482 | 0.6879 | 0.071* |

| | | | | |
|---|---|---|---|---|
| C13 | −0.0299 (3) | 0.4945 (9) | 0.66109 (10) | 0.0574 (12) |
| H13 | −0.0168 | 0.633 | 0.6767 | 0.069* |
| C14 | 0.0070 (2) | 0.4649 (8) | 0.63144 (10) | 0.0439 (10) |
| H14 | 0.0451 | 0.5798 | 0.6273 | 0.053* |
| C15 | 0.3338 (2) | 0.6863 (7) | 0.31213 (10) | 0.0382 (9) |
| C16 | 0.3837 (2) | 0.4959 (9) | 0.30577 (11) | 0.0517 (11) |
| H16 | 0.401 | 0.3772 | 0.3235 | 0.062* |
| C17 | 0.4088 (3) | 0.4791 (11) | 0.27288 (13) | 0.0676 (14) |
| H17 | 0.4425 | 0.3479 | 0.2685 | 0.081* |
| C18 | 0.3837 (3) | 0.6570 (11) | 0.24667 (12) | 0.0695 (15) |
| H18 | 0.4011 | 0.6476 | 0.2247 | 0.083* |
| C19 | 0.3336 (3) | 0.8462 (11) | 0.25299 (13) | 0.0738 (16) |
| H19 | 0.3157 | 0.9633 | 0.2352 | 0.089* |
| C20 | 0.3091 (3) | 0.8644 (9) | 0.28602 (12) | 0.0565 (12) |
| H20 | 0.2759 | 0.9971 | 0.2905 | 0.068* |
| N1 | 0.02190 (19) | 0.2112 (6) | 0.57763 (8) | 0.0381 (8) |
| H1N | 0.029 (2) | 0.055 (6) | 0.5713 (11) | 0.046* |
| N2 | 0.3100 (2) | 0.7191 (6) | 0.34624 (9) | 0.0405 (8) |
| H2N | 0.302 (2) | 0.868 (6) | 0.3547 (11) | 0.049* |
| O1 | 0.04456 (18) | 0.6348 (5) | 0.56139 (8) | 0.0503 (8) |
| O2 | 0.2948 (2) | 0.2890 (6) | 0.36057 (9) | 0.0652 (10) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.041 (2) | 0.029 (2) | 0.038 (2) | 0.0025 (17) | 0.0096 (17) | −0.0019 (17) |
| C2 | 0.050 (2) | 0.032 (2) | 0.038 (2) | −0.0012 (18) | 0.0144 (18) | −0.0054 (17) |
| C3 | 0.046 (2) | 0.037 (2) | 0.038 (2) | −0.0056 (18) | 0.0141 (17) | −0.0075 (17) |
| C4 | 0.044 (2) | 0.038 (2) | 0.039 (2) | −0.0018 (18) | 0.0125 (17) | −0.0048 (17) |
| C5 | 0.052 (2) | 0.038 (2) | 0.037 (2) | −0.0057 (19) | 0.0163 (18) | −0.0080 (18) |
| C6 | 0.055 (2) | 0.031 (2) | 0.042 (2) | −0.0081 (18) | 0.0166 (19) | −0.0062 (17) |
| C7 | 0.051 (2) | 0.033 (2) | 0.042 (2) | −0.0046 (19) | 0.0131 (19) | −0.0038 (18) |
| C8 | 0.050 (2) | 0.026 (2) | 0.044 (2) | −0.0011 (18) | 0.0215 (19) | −0.0072 (17) |
| C9 | 0.039 (2) | 0.0295 (19) | 0.0347 (19) | 0.0036 (17) | 0.0069 (16) | 0.0021 (15) |
| C10 | 0.057 (3) | 0.043 (2) | 0.039 (2) | −0.007 (2) | 0.0131 (19) | −0.0037 (18) |
| C11 | 0.060 (3) | 0.058 (3) | 0.056 (3) | 0.002 (2) | 0.029 (2) | 0.011 (2) |
| C12 | 0.079 (3) | 0.062 (3) | 0.042 (2) | 0.013 (3) | 0.030 (2) | 0.005 (2) |
| C13 | 0.089 (3) | 0.047 (3) | 0.037 (2) | 0.005 (3) | 0.011 (2) | −0.009 (2) |
| C14 | 0.051 (2) | 0.040 (2) | 0.041 (2) | −0.0034 (19) | 0.0109 (19) | −0.0051 (19) |
| C15 | 0.046 (2) | 0.030 (2) | 0.041 (2) | −0.0092 (17) | 0.0134 (18) | −0.0034 (17) |
| C16 | 0.060 (3) | 0.049 (2) | 0.050 (2) | 0.008 (2) | 0.021 (2) | 0.002 (2) |
| C17 | 0.081 (3) | 0.060 (3) | 0.070 (3) | 0.005 (3) | 0.042 (3) | −0.009 (3) |
| C18 | 0.102 (4) | 0.066 (3) | 0.046 (3) | −0.018 (3) | 0.035 (3) | −0.009 (3) |
| C19 | 0.113 (5) | 0.063 (3) | 0.047 (3) | −0.005 (3) | 0.019 (3) | 0.013 (3) |
| C20 | 0.072 (3) | 0.042 (3) | 0.058 (3) | 0.002 (2) | 0.017 (2) | 0.004 (2) |
| N1 | 0.0527 (19) | 0.0262 (16) | 0.0384 (17) | −0.0009 (15) | 0.0174 (15) | −0.0018 (14) |
| N2 | 0.054 (2) | 0.0263 (17) | 0.0446 (19) | −0.0037 (15) | 0.0198 (16) | −0.0016 (15) |
| O1 | 0.072 (2) | 0.0293 (15) | 0.0548 (18) | 0.0002 (14) | 0.0316 (16) | −0.0006 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O2 | 0.110 (3) | 0.0280 (16) | 0.067 (2) | −0.0056 (17) | 0.051 (2) | −0.0043 (14) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.229 (5) | C9—N1 | 1.423 (5) |
| C1—N1 | 1.350 (5) | C10—C11 | 1.386 (6) |
| C1—C2 | 1.508 (5) | C10—H10 | 0.93 |
| C2—C3 | 1.510 (5) | C11—C12 | 1.368 (7) |
| C2—H2A | 0.97 | C11—H11 | 0.93 |
| C2—H2B | 0.97 | C12—C13 | 1.366 (7) |
| C3—C4 | 1.512 (5) | C12—H12 | 0.93 |
| C3—H3A | 0.97 | C13—C14 | 1.388 (6) |
| C3—H3B | 0.97 | C13—H13 | 0.93 |
| C4—C5 | 1.513 (5) | C14—H14 | 0.93 |
| C4—H4A | 0.97 | C15—C16 | 1.362 (6) |
| C4—H4B | 0.97 | C15—C20 | 1.377 (6) |
| C5—C6 | 1.514 (5) | C15—N2 | 1.427 (5) |
| C5—H5A | 0.97 | C16—C17 | 1.385 (6) |
| C5—H5B | 0.97 | C16—H16 | 0.93 |
| C6—C7 | 1.509 (5) | C17—C18 | 1.381 (7) |
| C6—H6A | 0.97 | C17—H17 | 0.93 |
| C6—H6B | 0.97 | C18—C19 | 1.360 (8) |
| C7—C8 | 1.512 (5) | C18—H18 | 0.93 |
| C7—H7A | 0.97 | C19—C20 | 1.387 (7) |
| C7—H7B | 0.97 | C19—H19 | 0.93 |
| C8—O2 | 1.225 (5) | C20—H20 | 0.93 |
| C8—N2 | 1.342 (5) | N1—H1N | 0.84 (3) |
| C9—C10 | 1.380 (6) | N2—H2N | 0.84 (3) |
| C9—C14 | 1.381 (5) | | |
| O1—C1—N1 | 123.3 (3) | C10—C9—C14 | 119.9 (3) |
| O1—C1—C2 | 122.1 (3) | C10—C9—N1 | 117.5 (3) |
| N1—C1—C2 | 114.5 (3) | C14—C9—N1 | 122.5 (3) |
| C1—C2—C3 | 114.6 (3) | C9—C10—C11 | 120.7 (4) |
| C1—C2—H2A | 108.6 | C9—C10—H10 | 119.7 |
| C3—C2—H2A | 108.6 | C11—C10—H10 | 119.7 |
| C1—C2—H2B | 108.6 | C12—C11—C10 | 119.3 (4) |
| C3—C2—H2B | 108.6 | C12—C11—H11 | 120.3 |
| H2A—C2—H2B | 107.6 | C10—C11—H11 | 120.3 |
| C2—C3—C4 | 113.4 (3) | C13—C12—C11 | 120.1 (4) |
| C2—C3—H3A | 108.9 | C13—C12—H12 | 119.9 |
| C4—C3—H3A | 108.9 | C11—C12—H12 | 119.9 |
| C2—C3—H3B | 108.9 | C12—C13—C14 | 121.4 (4) |
| C4—C3—H3B | 108.9 | C12—C13—H13 | 119.3 |
| H3A—C3—H3B | 107.7 | C14—C13—H13 | 119.3 |
| C3—C4—C5 | 114.2 (3) | C9—C14—C13 | 118.5 (4) |
| C3—C4—H4A | 108.7 | C9—C14—H14 | 120.7 |
| C5—C4—H4A | 108.7 | C13—C14—H14 | 120.7 |
| C3—C4—H4B | 108.7 | C16—C15—C20 | 120.0 (4) |
| C5—C4—H4B | 108.7 | C16—C15—N2 | 121.5 (4) |

| | | | |
|---|---|---|---|
| H4A—C4—H4B | 107.6 | C20—C15—N2 | 118.4 (4) |
| C4—C5—C6 | 114.5 (3) | C15—C16—C17 | 120.0 (4) |
| C4—C5—H5A | 108.6 | C15—C16—H16 | 120 |
| C6—C5—H5A | 108.6 | C17—C16—H16 | 120 |
| C4—C5—H5B | 108.6 | C18—C17—C16 | 120.0 (5) |
| C6—C5—H5B | 108.6 | C18—C17—H17 | 120 |
| H5A—C5—H5B | 107.6 | C16—C17—H17 | 120 |
| C7—C6—C5 | 112.8 (3) | C19—C18—C17 | 119.9 (4) |
| C7—C6—H6A | 109 | C19—C18—H18 | 120 |
| C5—C6—H6A | 109 | C17—C18—H18 | 120 |
| C7—C6—H6B | 109 | C18—C19—C20 | 120.0 (5) |
| C5—C6—H6B | 109 | C18—C19—H19 | 120 |
| H6A—C6—H6B | 107.8 | C20—C19—H19 | 120 |
| C6—C7—C8 | 113.3 (3) | C15—C20—C19 | 120.1 (5) |
| C6—C7—H7A | 108.9 | C15—C20—H20 | 119.9 |
| C8—C7—H7A | 108.9 | C19—C20—H20 | 119.9 |
| C6—C7—H7B | 108.9 | C1—N1—C9 | 126.9 (3) |
| C8—C7—H7B | 108.9 | C1—N1—H1N | 113 (3) |
| H7A—C7—H7B | 107.7 | C9—N1—H1N | 120 (3) |
| O2—C8—N2 | 123.0 (4) | C8—N2—C15 | 126.8 (3) |
| O2—C8—C7 | 122.3 (4) | C8—N2—H2N | 110 (3) |
| N2—C8—C7 | 114.6 (3) | C15—N2—H2N | 123 (3) |
| O1—C1—C2—C3 | 23.9 (6) | C20—C15—C16—C17 | −0.9 (7) |
| N1—C1—C2—C3 | −159.8 (3) | N2—C15—C16—C17 | −176.4 (4) |
| C1—C2—C3—C4 | −173.8 (3) | C15—C16—C17—C18 | 0.7 (8) |
| C2—C3—C4—C5 | 179.0 (4) | C16—C17—C18—C19 | −1.0 (8) |
| C3—C4—C5—C6 | −178.1 (4) | C17—C18—C19—C20 | 1.7 (8) |
| C4—C5—C6—C7 | −179.4 (4) | C16—C15—C20—C19 | 1.5 (7) |
| C5—C6—C7—C8 | −178.9 (4) | N2—C15—C20—C19 | 177.1 (4) |
| C6—C7—C8—O2 | −29.1 (6) | C18—C19—C20—C15 | −1.9 (8) |
| C6—C7—C8—N2 | 152.7 (4) | O1—C1—N1—C9 | 1.5 (7) |
| C14—C9—C10—C11 | 1.7 (6) | C2—C1—N1—C9 | −174.8 (4) |
| N1—C9—C10—C11 | 178.2 (4) | C10—C9—N1—C1 | 145.5 (4) |
| C9—C10—C11—C12 | −0.6 (7) | C14—C9—N1—C1 | −38.0 (6) |
| C10—C11—C12—C13 | −0.2 (7) | O2—C8—N2—C15 | −1.4 (7) |
| C11—C12—C13—C14 | 0.0 (7) | C7—C8—N2—C15 | 176.8 (4) |
| C10—C9—C14—C13 | −2.0 (6) | C16—C15—N2—C8 | −42.2 (6) |
| N1—C9—C14—C13 | −178.3 (4) | C20—C15—N2—C8 | 142.3 (4) |
| C12—C13—C14—C9 | 1.1 (7) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1N···O1$^{i}$ | 0.84 (3) | 2.17 (3) | 3.004 (4) | 173 (4) |
| N2—H2N···O2$^{ii}$ | 0.84 (3) | 2.13 (3) | 2.937 (4) | 161 (4) |

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

**Fig. 1**

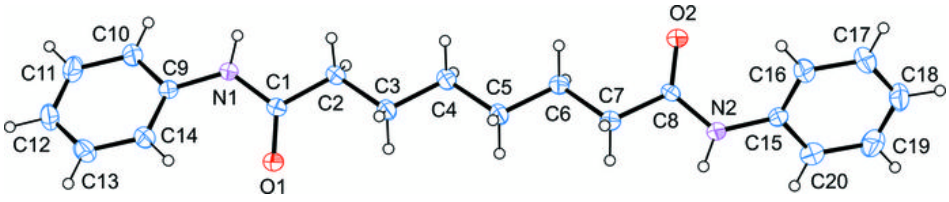
C10
C11
C9
N1
C1
C2
C3
C4
C5
C6
C7
C8
O2
N2
C17
C16
C18
C12
C14
C15
C19
C13
O1
C20

**Fig. 2**