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(E)-N-[2-(Biphenyl-4-ylvinyl)phenyl]-furan-2-carboxamide

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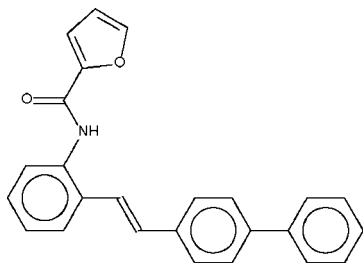
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.039; wR factor = 0.106; data-to-parameter ratio = 17.2.

In the title molecule, $\text{C}_{25}\text{H}_{19}\text{NO}_2$, the furyl ring is twisted by 46.3 (1)° with respect to the phenylene ring bearing the amido group. In the stilbene unit, the two phenylene rings (*i.e.* the rings connected through the $-\text{CH}=\text{CH}-$ fragment) are twisted by 59.2 (1)°; in the biphenylene unit, the two benzene rings are twisted by 35.5 (1)°. In the crystal structure, molecules are linked by an $\text{N}-\text{H}\cdots\text{O}_{\text{amido}}$ hydrogen bond into a zigzag chain running along the c axis.

Related literature

For the use of radical cations in heterocyclic synthesis, see: Thomas *et al.* (2004, 2008).



Experimental

Crystal data

$\text{C}_{25}\text{H}_{19}\text{NO}_2$

$M_r = 365.41$

Monoclinic, $P2_1/c$
 $a = 10.9271$ (2) Å
 $b = 19.7960$ (4) Å
 $c = 8.7969$ (1) Å
 $\beta = 92.374$ (1)°
 $V = 1901.25$ (6) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 100$ (2) K
 $0.40 \times 0.35 \times 0.15$ mm

Data collection

Bruker SMART APEX
diffractometer
Absorption correction: none
13179 measured reflections

4356 independent reflections
3681 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.106$
 $S = 1.04$
4356 reflections

253 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.30$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{N1}-\text{H1}\cdots\text{O2}^i$ | 0.88 | 2.05 | 2.903 (1) | 163 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2714).

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supplementary materials

Acta Cryst. (2008). E64, o2210 [doi:10.1107/S1600536808034569]

(*E*)-*N*-[2-(Biphenyl-4-ylvinyl)phenyl]furan-2-carboxamide

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Comment

In our earlier studies, we reported the synthesis of some stilbene carboxamides whose radical chemistry we investigated (Thomas *et al.*, 2004, 2008). In the present study, we have synthesized a new stilbene carboxamide that incorporates a furan unit (Scheme I, Fig. 1).

Experimental

N-(2-Iodophenyl)furan-2-carboxamide (0.37 g, 1.2 mmol) was dissolved in DMF (20 ml) under a nitrogen atmosphere. The solution was heated to 373 K. Palladium acetate (3.2 mg, 0.014 mmol) was added followed by triethylamine (0.65 ml, 4.7 mmol) and 4-vinylbiphenyl (0.20 g, 1.21 mmol). The mixture was further heated for an hour. The solution was cooled and then mixed with saturated sodium chloride. The organic compound was extracted with ethyl acetate. The ethyl acetate solution was dried with sodium sulfate. The solvent was evaporated and the product purified by column chromatography. Single crystals were obtained by recrystallization from petroleum ether/dichloromethane.

Refinement

Carbon- and nitrogen- bound H-atoms were placed in calculated positions (C—H 0.95, N—H 0.88 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U(\text{C},\text{N})$.

Figures

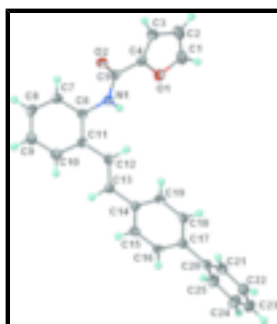


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $\text{C}_{25}\text{H}_{19}\text{NO}_2$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radii.

(*E*)-*N*-[2-(Biphenyl-4-ylvinyl)phenyl]furan-2-carboxamide

Crystal data

$\text{C}_{25}\text{H}_{19}\text{NO}_2$

$M_r = 365.41$

Monoclinic, $P2_1/c$

$F_{000} = 768$

$D_x = 1.277 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

supplementary materials

| | |
|---------------------------------|---|
| Hall symbol: -P 2ybc | $\lambda = 0.71073 \text{ \AA}$ |
| $a = 10.9271 (2) \text{ \AA}$ | Cell parameters from 5580 reflections |
| $b = 19.7960 (4) \text{ \AA}$ | $\theta = 2.5\text{--}28.2^\circ$ |
| $c = 8.7969 (1) \text{ \AA}$ | $\mu = 0.08 \text{ mm}^{-1}$ |
| $\beta = 92.374 (1)^\circ$ | $T = 100 (2) \text{ K}$ |
| $V = 1901.25 (6) \text{ \AA}^3$ | Prism, colorless |
| $Z = 4$ | $0.40 \times 0.35 \times 0.15 \text{ mm}$ |

Data collection

| | |
|--|--|
| Bruker SMART APEX diffractometer | 3681 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{\text{int}} = 0.022$ |
| Monochromator: graphite | $\theta_{\text{max}} = 27.5^\circ$ |
| $T = 100(2) \text{ K}$ | $\theta_{\text{min}} = 1.9^\circ$ |
| ω scans | $h = -14 \rightarrow 13$ |
| Absorption correction: None | $k = -25 \rightarrow 25$ |
| 13179 measured reflections | $l = -11 \rightarrow 11$ |
| 4356 independent reflections | |

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-atom parameters constrained |
| $wR(F^2) = 0.106$ | $w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.6489P]$ |
| $S = 1.04$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 4356 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 253 parameters | $\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$ |
| | Extinction correction: none |

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.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|-------------|-------------|--------------|----------------------------------|
| O1 | 0.69066 (8) | 0.17866 (4) | 0.88070 (9) | 0.0218 (2) |
| O2 | 0.56344 (8) | 0.18549 (4) | 0.50228 (9) | 0.01969 (19) |
| N1 | 0.52573 (9) | 0.25519 (5) | 0.70226 (11) | 0.0173 (2) |

| | | | | |
|-----|--------------|-------------|--------------|------------|
| H1 | 0.5441 | 0.2651 | 0.7981 | 0.021* |
| C1 | 0.76833 (12) | 0.13051 (7) | 0.93850 (15) | 0.0263 (3) |
| H1A | 0.8056 | 0.1316 | 1.0380 | 0.032* |
| C2 | 0.78542 (12) | 0.08127 (7) | 0.83672 (16) | 0.0274 (3) |
| H2 | 0.8347 | 0.0421 | 0.8510 | 0.033* |
| C3 | 0.71470 (11) | 0.09950 (6) | 0.70252 (15) | 0.0221 (3) |
| H3 | 0.7080 | 0.0751 | 0.6096 | 0.027* |
| C4 | 0.65936 (11) | 0.15860 (6) | 0.73503 (13) | 0.0171 (2) |
| C5 | 0.57830 (10) | 0.20106 (6) | 0.63762 (13) | 0.0164 (2) |
| C6 | 0.44068 (11) | 0.29656 (6) | 0.61664 (13) | 0.0168 (2) |
| C7 | 0.34268 (11) | 0.26554 (6) | 0.53871 (14) | 0.0205 (3) |
| H7 | 0.3306 | 0.2183 | 0.5488 | 0.025* |
| C8 | 0.26273 (11) | 0.30299 (7) | 0.44657 (14) | 0.0228 (3) |
| H8 | 0.1971 | 0.2814 | 0.3914 | 0.027* |
| C9 | 0.27890 (12) | 0.37245 (7) | 0.43514 (14) | 0.0237 (3) |
| H9 | 0.2252 | 0.3984 | 0.3707 | 0.028* |
| C10 | 0.37337 (11) | 0.40363 (6) | 0.51779 (14) | 0.0213 (3) |
| H10 | 0.3821 | 0.4513 | 0.5114 | 0.026* |
| C11 | 0.45663 (11) | 0.36676 (6) | 0.61073 (13) | 0.0172 (2) |
| C12 | 0.55685 (11) | 0.40039 (6) | 0.69725 (13) | 0.0176 (2) |
| H12 | 0.6298 | 0.3755 | 0.7193 | 0.021* |
| C13 | 0.55134 (11) | 0.46414 (6) | 0.74683 (13) | 0.0182 (2) |
| H13 | 0.4776 | 0.4882 | 0.7240 | 0.022* |
| C14 | 0.64845 (11) | 0.50049 (6) | 0.83315 (13) | 0.0168 (2) |
| C15 | 0.61548 (11) | 0.55136 (6) | 0.93372 (13) | 0.0178 (2) |
| H15 | 0.5313 | 0.5613 | 0.9446 | 0.021* |
| C16 | 0.70291 (11) | 0.58746 (6) | 1.01760 (13) | 0.0179 (2) |
| H16 | 0.6778 | 0.6198 | 1.0896 | 0.021* |
| C17 | 0.82804 (11) | 0.57700 (6) | 0.99805 (13) | 0.0173 (2) |
| C18 | 0.86116 (11) | 0.52600 (6) | 0.89750 (13) | 0.0185 (2) |
| H18 | 0.9454 | 0.5175 | 0.8830 | 0.022* |
| C19 | 0.77344 (11) | 0.48767 (6) | 0.81860 (13) | 0.0184 (2) |
| H19 | 0.7984 | 0.4523 | 0.7539 | 0.022* |
| C20 | 0.91995 (11) | 0.62106 (6) | 1.07784 (13) | 0.0177 (2) |
| C21 | 1.02722 (11) | 0.64044 (6) | 1.00799 (14) | 0.0204 (3) |
| H21 | 1.0433 | 0.6235 | 0.9098 | 0.025* |
| C22 | 1.11036 (11) | 0.68399 (6) | 1.07977 (14) | 0.0224 (3) |
| H22 | 1.1832 | 0.6962 | 1.0312 | 0.027* |
| C23 | 1.08758 (12) | 0.70986 (7) | 1.22235 (15) | 0.0237 (3) |
| H23 | 1.1436 | 0.7405 | 1.2706 | 0.028* |
| C24 | 0.98214 (13) | 0.69059 (7) | 1.29408 (15) | 0.0274 (3) |
| H24 | 0.9665 | 0.7078 | 1.3922 | 0.033* |
| C25 | 0.89957 (11) | 0.64639 (7) | 1.22295 (14) | 0.0234 (3) |
| H25 | 0.8282 | 0.6332 | 1.2735 | 0.028* |

Atomic displacement parameters (\AA^2)

U^{11}

U^{22}

U^{33}

U^{12}

U^{13}

U^{23}

supplementary materials

| | | | | | | |
|-----|------------|------------|------------|-------------|-------------|-------------|
| O1 | 0.0244 (4) | 0.0254 (5) | 0.0155 (4) | -0.0007 (4) | -0.0020 (3) | 0.0003 (3) |
| O2 | 0.0252 (4) | 0.0194 (4) | 0.0144 (4) | 0.0002 (3) | -0.0003 (3) | -0.0011 (3) |
| N1 | 0.0219 (5) | 0.0164 (5) | 0.0134 (4) | -0.0005 (4) | -0.0018 (4) | -0.0020 (4) |
| C1 | 0.0239 (6) | 0.0339 (7) | 0.0208 (6) | 0.0012 (5) | -0.0029 (5) | 0.0074 (5) |
| C2 | 0.0232 (6) | 0.0279 (7) | 0.0311 (7) | 0.0034 (5) | 0.0011 (5) | 0.0086 (6) |
| C3 | 0.0225 (6) | 0.0205 (6) | 0.0236 (6) | -0.0005 (5) | 0.0026 (5) | -0.0004 (5) |
| C4 | 0.0184 (5) | 0.0181 (6) | 0.0148 (5) | -0.0039 (4) | 0.0013 (4) | 0.0001 (4) |
| C5 | 0.0177 (5) | 0.0147 (5) | 0.0168 (5) | -0.0036 (4) | 0.0020 (4) | 0.0009 (4) |
| C6 | 0.0195 (5) | 0.0177 (6) | 0.0133 (5) | 0.0009 (4) | 0.0010 (4) | -0.0010 (4) |
| C7 | 0.0231 (6) | 0.0183 (6) | 0.0202 (6) | -0.0015 (5) | 0.0011 (5) | -0.0032 (5) |
| C8 | 0.0209 (6) | 0.0283 (7) | 0.0189 (6) | -0.0029 (5) | -0.0021 (5) | -0.0039 (5) |
| C9 | 0.0242 (6) | 0.0278 (7) | 0.0188 (6) | 0.0017 (5) | -0.0037 (5) | 0.0041 (5) |
| C10 | 0.0252 (6) | 0.0188 (6) | 0.0198 (6) | -0.0007 (5) | 0.0005 (5) | 0.0030 (5) |
| C11 | 0.0199 (5) | 0.0188 (6) | 0.0131 (5) | -0.0010 (4) | 0.0019 (4) | 0.0003 (4) |
| C12 | 0.0188 (5) | 0.0180 (6) | 0.0161 (5) | -0.0009 (4) | 0.0008 (4) | 0.0025 (4) |
| C13 | 0.0188 (5) | 0.0178 (6) | 0.0177 (6) | -0.0010 (4) | 0.0002 (4) | 0.0016 (4) |
| C14 | 0.0202 (6) | 0.0132 (5) | 0.0170 (5) | -0.0014 (4) | -0.0006 (4) | 0.0035 (4) |
| C15 | 0.0175 (5) | 0.0156 (5) | 0.0205 (6) | 0.0002 (4) | 0.0015 (4) | 0.0028 (4) |
| C16 | 0.0215 (6) | 0.0131 (5) | 0.0191 (6) | 0.0003 (4) | 0.0023 (4) | 0.0006 (4) |
| C17 | 0.0200 (6) | 0.0149 (5) | 0.0167 (5) | -0.0002 (4) | -0.0007 (4) | 0.0035 (4) |
| C18 | 0.0176 (5) | 0.0181 (6) | 0.0198 (6) | 0.0022 (4) | 0.0001 (4) | 0.0023 (5) |
| C19 | 0.0228 (6) | 0.0147 (5) | 0.0179 (6) | 0.0020 (4) | 0.0014 (4) | 0.0002 (4) |
| C20 | 0.0188 (5) | 0.0147 (5) | 0.0195 (6) | 0.0013 (4) | -0.0020 (4) | 0.0013 (4) |
| C21 | 0.0213 (6) | 0.0205 (6) | 0.0195 (6) | 0.0009 (5) | 0.0012 (5) | -0.0007 (5) |
| C22 | 0.0194 (6) | 0.0239 (6) | 0.0240 (6) | -0.0029 (5) | 0.0012 (5) | 0.0031 (5) |
| C23 | 0.0235 (6) | 0.0244 (6) | 0.0228 (6) | -0.0053 (5) | -0.0039 (5) | -0.0015 (5) |
| C24 | 0.0279 (7) | 0.0340 (7) | 0.0202 (6) | -0.0058 (6) | 0.0010 (5) | -0.0061 (5) |
| C25 | 0.0216 (6) | 0.0280 (7) | 0.0208 (6) | -0.0051 (5) | 0.0024 (5) | -0.0005 (5) |

Geometric parameters (Å, °)

| | | | |
|--------|-------------|---------|-------------|
| O1—C1 | 1.3607 (16) | C12—H12 | 0.9500 |
| O1—C4 | 1.3714 (14) | C13—C14 | 1.4676 (16) |
| O2—C5 | 1.2340 (14) | C13—H13 | 0.9500 |
| N1—C5 | 1.3523 (15) | C14—C15 | 1.3975 (16) |
| N1—C6 | 1.4295 (15) | C14—C19 | 1.4002 (16) |
| N1—H1 | 0.8800 | C15—C16 | 1.3818 (17) |
| C1—C2 | 1.342 (2) | C15—H15 | 0.9500 |
| C1—H1A | 0.9500 | C16—C17 | 1.4005 (16) |
| C2—C3 | 1.4302 (19) | C16—H16 | 0.9500 |
| C2—H2 | 0.9500 | C17—C18 | 1.3996 (17) |
| C3—C4 | 1.3528 (17) | C17—C20 | 1.4845 (16) |
| C3—H3 | 0.9500 | C18—C19 | 1.3860 (17) |
| C4—C5 | 1.4706 (16) | C18—H18 | 0.9500 |
| C6—C7 | 1.3903 (17) | C19—H19 | 0.9500 |
| C6—C11 | 1.4019 (16) | C20—C25 | 1.3979 (17) |
| C7—C8 | 1.3825 (18) | C20—C21 | 1.3994 (16) |
| C7—H7 | 0.9500 | C21—C22 | 1.3856 (18) |
| C8—C9 | 1.3904 (19) | C21—H21 | 0.9500 |

| | | | |
|-------------|-------------|-----------------|-------------|
| C8—H8 | 0.9500 | C22—C23 | 1.3869 (18) |
| C9—C10 | 1.3832 (18) | C22—H22 | 0.9500 |
| C9—H9 | 0.9500 | C23—C24 | 1.3897 (18) |
| C10—C11 | 1.4026 (17) | C23—H23 | 0.9500 |
| C10—H10 | 0.9500 | C24—C25 | 1.3872 (18) |
| C11—C12 | 1.4672 (16) | C24—H24 | 0.9500 |
| C12—C13 | 1.3373 (17) | C25—H25 | 0.9500 |
| C1—O1—C4 | 105.89 (10) | C12—C13—C14 | 126.16 (11) |
| C5—N1—C6 | 120.70 (10) | C12—C13—H13 | 116.9 |
| C5—N1—H1 | 119.6 | C14—C13—H13 | 116.9 |
| C6—N1—H1 | 119.6 | C15—C14—C19 | 117.80 (11) |
| C2—C1—O1 | 111.19 (11) | C15—C14—C13 | 118.76 (10) |
| C2—C1—H1A | 124.4 | C19—C14—C13 | 123.43 (11) |
| O1—C1—H1A | 124.4 | C16—C15—C14 | 121.34 (11) |
| C1—C2—C3 | 106.39 (12) | C16—C15—H15 | 119.3 |
| C1—C2—H2 | 126.8 | C14—C15—H15 | 119.3 |
| C3—C2—H2 | 126.8 | C15—C16—C17 | 120.99 (11) |
| C4—C3—C2 | 105.94 (12) | C15—C16—H16 | 119.5 |
| C4—C3—H3 | 127.0 | C17—C16—H16 | 119.5 |
| C2—C3—H3 | 127.0 | C18—C17—C16 | 117.61 (11) |
| C3—C4—O1 | 110.59 (11) | C18—C17—C20 | 122.35 (10) |
| C3—C4—C5 | 129.40 (11) | C16—C17—C20 | 119.99 (10) |
| O1—C4—C5 | 119.99 (10) | C19—C18—C17 | 121.32 (11) |
| O2—C5—N1 | 124.22 (11) | C19—C18—H18 | 119.3 |
| O2—C5—C4 | 118.13 (10) | C17—C18—H18 | 119.3 |
| N1—C5—C4 | 117.65 (10) | C18—C19—C14 | 120.80 (11) |
| C7—C6—C11 | 120.92 (11) | C18—C19—H19 | 119.6 |
| C7—C6—N1 | 118.52 (10) | C14—C19—H19 | 119.6 |
| C11—C6—N1 | 120.55 (10) | C25—C20—C21 | 118.08 (11) |
| C8—C7—C6 | 120.50 (11) | C25—C20—C17 | 120.81 (10) |
| C8—C7—H7 | 119.8 | C21—C20—C17 | 121.06 (10) |
| C6—C7—H7 | 119.8 | C22—C21—C20 | 121.05 (11) |
| C7—C8—C9 | 119.57 (12) | C22—C21—H21 | 119.5 |
| C7—C8—H8 | 120.2 | C20—C21—H21 | 119.5 |
| C9—C8—H8 | 120.2 | C21—C22—C23 | 120.20 (11) |
| C10—C9—C8 | 119.85 (12) | C21—C22—H22 | 119.9 |
| C10—C9—H9 | 120.1 | C23—C22—H22 | 119.9 |
| C8—C9—H9 | 120.1 | C22—C23—C24 | 119.50 (12) |
| C9—C10—C11 | 121.74 (11) | C22—C23—H23 | 120.2 |
| C9—C10—H10 | 119.1 | C24—C23—H23 | 120.2 |
| C11—C10—H10 | 119.1 | C25—C24—C23 | 120.29 (12) |
| C6—C11—C10 | 117.32 (11) | C25—C24—H24 | 119.9 |
| C6—C11—C12 | 121.45 (11) | C23—C24—H24 | 119.9 |
| C10—C11—C12 | 121.22 (11) | C24—C25—C20 | 120.85 (11) |
| C13—C12—C11 | 123.68 (11) | C24—C25—H25 | 119.6 |
| C13—C12—H12 | 118.2 | C20—C25—H25 | 119.6 |
| C11—C12—H12 | 118.2 | | |
| C4—O1—C1—C2 | -0.80 (14) | C10—C11—C12—C13 | 28.50 (17) |

supplementary materials

| | | | |
|----------------|--------------|-----------------|--------------|
| O1—C1—C2—C3 | 0.80 (15) | C11—C12—C13—C14 | -179.77 (10) |
| C1—C2—C3—C4 | -0.48 (14) | C12—C13—C14—C15 | -150.97 (12) |
| C2—C3—C4—O1 | 0.00 (14) | C12—C13—C14—C19 | 30.06 (18) |
| C2—C3—C4—C5 | 178.41 (11) | C19—C14—C15—C16 | -0.73 (17) |
| C1—O1—C4—C3 | 0.47 (13) | C13—C14—C15—C16 | -179.76 (10) |
| C1—O1—C4—C5 | -178.11 (10) | C14—C15—C16—C17 | 3.81 (17) |
| C6—N1—C5—O2 | 4.14 (17) | C15—C16—C17—C18 | -3.75 (17) |
| C6—N1—C5—C4 | -176.54 (10) | C15—C16—C17—C20 | 173.84 (10) |
| C3—C4—C5—O2 | -6.48 (18) | C16—C17—C18—C19 | 0.74 (17) |
| O1—C4—C5—O2 | 171.80 (10) | C20—C17—C18—C19 | -176.79 (11) |
| C3—C4—C5—N1 | 174.16 (12) | C17—C18—C19—C14 | 2.28 (18) |
| O1—C4—C5—N1 | -7.56 (15) | C15—C14—C19—C18 | -2.28 (17) |
| C5—N1—C6—C7 | 51.61 (15) | C13—C14—C19—C18 | 176.70 (11) |
| C5—N1—C6—C11 | -127.90 (12) | C18—C17—C20—C25 | -148.23 (12) |
| C11—C6—C7—C8 | 3.72 (17) | C16—C17—C20—C25 | 34.29 (17) |
| N1—C6—C7—C8 | -175.79 (10) | C18—C17—C20—C21 | 34.12 (17) |
| C6—C7—C8—C9 | -1.66 (18) | C16—C17—C20—C21 | -143.35 (12) |
| C7—C8—C9—C10 | -1.08 (18) | C25—C20—C21—C22 | -0.62 (18) |
| C8—C9—C10—C11 | 1.85 (18) | C17—C20—C21—C22 | 177.09 (11) |
| C7—C6—C11—C10 | -2.91 (16) | C20—C21—C22—C23 | -0.77 (19) |
| N1—C6—C11—C10 | 176.59 (10) | C21—C22—C23—C24 | 1.4 (2) |
| C7—C6—C11—C12 | 177.55 (10) | C22—C23—C24—C25 | -0.7 (2) |
| N1—C6—C11—C12 | -2.95 (16) | C23—C24—C25—C20 | -0.7 (2) |
| C9—C10—C11—C6 | 0.14 (17) | C21—C20—C25—C24 | 1.35 (19) |
| C9—C10—C11—C12 | 179.68 (11) | C17—C20—C25—C24 | -176.37 (12) |
| C6—C11—C12—C13 | -151.98 (12) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------|-------|-------------|-------------|---------------|
| $N1-H1\cdots O2^i$ | 0.88 | 2.05 | 2.903 (1) | 163 |

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

Fig. 1

