

## organic compounds

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N-[4-(4-Nitrophenoxy)phenyl]-  
propionamideAsifa Nigar,<sup>a</sup> Zareen Akhter,<sup>a\*</sup> Michael Bolte,<sup>b</sup>  
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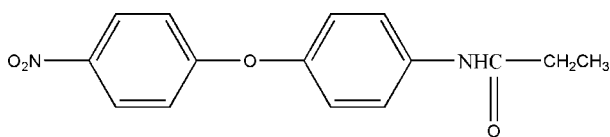
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.096; data-to-parameter ratio = 14.3.

The title compound,  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_4$ , is an important intermediate for the synthesis of thermotropic liquid crystals. The dihedral angle between the two aromatic rings is  $84.29(4)^\circ$ . An  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond connects the molecules into chains running along the  $b$  axis. In addition, the crystal packing is stabilized by weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds.

## Related literature

For background on liquid crystals, see: Bahadur (1992); Collings (1990); Collings & Hird (1997). For bond lengths and angles in organic compounds, see: Allen *et al.* (1995). For related literature, see: Akhter *et al.* (2007); Cârlescu *et al.* (2005).



## Experimental

## Crystal data

 $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_4$  $M_r = 286.28$ Monoclinic,  $P2_1/n$  $a = 14.8597(14)$  Å $b = 5.2400(3)$  Å $c = 17.9034(16)$  Å $\beta = 101.875(7)^\circ$  $V = 1364.21(19)$  Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 173(2)$  K $0.37 \times 0.28 \times 0.19$  mm

## Data collection

Stoe IPDSII diffractometer  
Absorption correction: none  
16399 measured reflections2788 independent reflections  
2347 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.048$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.036$  $wR(F^2) = 0.096$  $S = 1.03$ 

2788 reflections

195 parameters

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.28$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.19$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$                                       | $D-H$      | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|------------|-------------|-------------|---------------|
| $\text{N1}-\text{H1}\cdots\text{O1}^{\text{i}}$     | 0.825 (17) | 2.255 (17)  | 3.0306 (13) | 156.7 (15)    |
| $\text{C25}-\text{H25}\cdots\text{O3}^{\text{ii}}$  | 0.95       | 2.42        | 3.2082 (17) | 140           |
| $\text{C23}-\text{H23}\cdots\text{O4}^{\text{iii}}$ | 0.95       | 2.53        | 3.3400 (16) | 144           |

Symmetry codes: (i)  $x, y-1, z$ ; (ii)  $-x, -y+2, -z+2$ ; (iii)  $-x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$ .

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2199).

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**supplementary materials**

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## ***N*-[4-(4-Nitrophenoxy)phenyl]propionamide**

**A. Nigar, Z. Akhter, M. Bolte, H. M. Siddiqi and R. Hussain**

### **Comment**

Liquid crystals are materials which exhibit phases where molecular order is intermediate between that of an ordered solid and a disordered liquid. They represent the combined properties of both the crystalline state (*e.g.* optical and electrical anisotropy) and the liquid state (*e.g.* molecular mobility and fluidity). The two major classes of liquid crystals are thermotropic and lyotropic, which can be distinguished by the mechanism that drive their self-organization. Background information on liquid crystals and their various applications were surveyed, for example, by Collings (1990), Bahadur (1992), and Collings & Hird (1997). One of the basic characteristics for the establishment of the mesophase is the ratio of rigid and flexible portions in the main structure (Cârlescu *et al.*, 2005). Therefore such type of precursors can be used to study structure property relationship of the liquid crystalline materials.

The crystal structure of the compound reported here is an important intermediate for the synthesis of thermotropic liquid crystals (Akhter *et al.*, 2007).

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1995) and angles are within normal ranges.

The dihedral angle between the two aromatic rings is 84.29 (4)°. An N—H···O hydrogen bond connects the molecules to chains running along the *b* axis. In addition, the crystal packing is stabilized by weak C—H···O hydrogen bonds.

### **Experimental**

A mixture of 5.046 g (50 mmol) 4-aminophenol, 6.91 g (50 mmol) anhydrous K<sub>2</sub>CO<sub>3</sub> and 5.3 ml (50 mmol) 4-nitrofluorobenzene in 70 ml DMF was heated at 373 K for 18 h in an inert atmosphere. After cooling to room temperature, the reaction mixture was poured into 800 ml of water to yield a yellow solid. The product was filtered, dried and then re-crystallized from *n*-hexane (yield 86%). In a second step, propanoic acid and thionylchloride were refluxed in equimolar amounts for 30 min before evaporating excessive thionylchloride with a vacuum pump. The above prepared 4-[4-nitrophenoxy]aniline was then added to the propanoyl chloride solution in dry THF. 1 ml of triethylamine was also added for 1 g of 4-[4-nitrophenoxy]aniline and refluxed for 2 h under inert conditions. The reaction mixture was allowed to stand at room temperature overnight and filtered off the salt formed. The filtrate was evaporated using a rotary evaporator, and the crude product obtained was re-crystallized from toluene (yield 76%, m.p. 416 K).

### **Refinement**

All H atoms could be located from difference Fourier maps. Except the amino H atom that was freely refined, all other H atoms were refined using a riding model with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$  and distance restraints of C—H(aromatic) = 0.95 Å, C—H(methyl) = 0.98 Å and C—H(methylene) = 0.99 Å, respectively.

## Figures

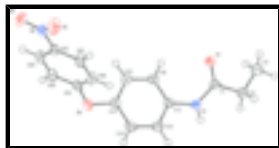


Fig. 1. The molecule of the title compound with atom labelling and displacement ellipsoids drawn at the 50% probability level. H atoms are given as spheres of arbitrary radius.

## *N*-[4-(4-Nitrophenoxy)phenyl]propionamide

### Crystal data

$C_{15}H_{14}N_2O_4$

$M_r = 286.28$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 14.8597$  (14) Å

$b = 5.2400$  (3) Å

$c = 17.9034$  (16) Å

$\beta = 101.875$  (7)°

$V = 1364.21$  (19) Å<sup>3</sup>

$Z = 4$

$F_{000} = 600$

$D_x = 1.394$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 14480 reflections

$\theta = 3.5$ – $26.6$ °

$\mu = 0.10$  mm<sup>-1</sup>

$T = 173$  (2) K

Plate, yellow

$0.37 \times 0.28 \times 0.19$  mm

### Data collection

Stoe IPDSII  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 173$ (2) K

$\omega$  scans

Absorption correction: none

16399 measured reflections

2788 independent reflections

2347 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.048$

$\theta_{max} = 26.4$ °

$\theta_{min} = 3.5$ °

$h = -18 \rightarrow 18$

$k = -6 \rightarrow 6$

$l = -22 \rightarrow 22$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.096$

$S = 1.03$

2788 reflections

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.2968P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.28$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.19$  e Å<sup>-3</sup>

195 parameters

Extinction correction: SHELXL97 (Sheldrick, 2008),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0097 (15)

Secondary atom site location: difference Fourier map

### 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 ( $\text{\AA}^2$ )

|     | <i>x</i>     | <i>y</i>     | <i>z</i>    | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|-------------|----------------------------------|
| N1  | 0.49215 (7)  | 0.2717 (2)   | 0.90078 (6) | 0.0246 (2)                       |
| H1  | 0.5157 (11)  | 0.129 (3)    | 0.9083 (9)  | 0.033 (4)*                       |
| N2  | -0.13564 (7) | 0.9965 (2)   | 0.86242 (7) | 0.0307 (3)                       |
| O1  | 0.52173 (6)  | 0.69920 (16) | 0.90359 (6) | 0.0319 (2)                       |
| O2  | 0.10753 (6)  | 0.21455 (17) | 0.82463 (6) | 0.0321 (2)                       |
| O3  | -0.12604 (8) | 1.1019 (2)   | 0.92505 (7) | 0.0495 (3)                       |
| O4  | -0.19763 (7) | 1.0515 (2)   | 0.80818 (6) | 0.0418 (3)                       |
| C1  | 0.54954 (8)  | 0.4769 (2)   | 0.91080 (7) | 0.0234 (3)                       |
| C2  | 0.65154 (9)  | 0.4133 (2)   | 0.93362 (8) | 0.0290 (3)                       |
| H2A | 0.6700       | 0.4115       | 0.9900      | 0.035*                           |
| H2B | 0.6620       | 0.2402       | 0.9149      | 0.035*                           |
| C3  | 0.71154 (9)  | 0.6026 (3)   | 0.90187 (9) | 0.0352 (3)                       |
| H3A | 0.7763       | 0.5540       | 0.9183      | 0.053*                           |
| H3B | 0.7023       | 0.7740       | 0.9209      | 0.053*                           |
| H3C | 0.6947       | 0.6019       | 0.8460      | 0.053*                           |
| C11 | 0.39403 (8)  | 0.2759 (2)   | 0.88371 (7) | 0.0226 (3)                       |
| C12 | 0.34820 (9)  | 0.0773 (2)   | 0.91224 (8) | 0.0291 (3)                       |
| H12 | 0.3826       | -0.0495      | 0.9437      | 0.035*                           |
| C13 | 0.25238 (9)  | 0.0633 (2)   | 0.89496 (8) | 0.0302 (3)                       |
| H13 | 0.2215       | -0.0714      | 0.9148      | 0.036*                           |
| C14 | 0.20289 (8)  | 0.2483 (2)   | 0.84859 (7) | 0.0250 (3)                       |
| C15 | 0.24723 (9)  | 0.4488 (2)   | 0.82019 (7) | 0.0270 (3)                       |
| H15 | 0.2124       | 0.5757       | 0.7890      | 0.032*                           |
| C16 | 0.34320 (9)  | 0.4629 (2)   | 0.83775 (7) | 0.0258 (3)                       |
| H16 | 0.3738       | 0.5994       | 0.8185      | 0.031*                           |
| C21 | 0.05086 (8)  | 0.4152 (2)   | 0.83521 (7) | 0.0251 (3)                       |
| C22 | -0.02514 (9) | 0.4618 (3)   | 0.77680 (7) | 0.0309 (3)                       |
| H22 | -0.0347      | 0.3634       | 0.7313      | 0.037*                           |

## supplementary materials

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|     |              |            |             |            |
|-----|--------------|------------|-------------|------------|
| C23 | -0.08678 (9) | 0.6532 (3) | 0.78568 (7) | 0.0306 (3) |
| H23 | -0.1389      | 0.6875     | 0.7464      | 0.037*     |
| C24 | -0.07090 (8) | 0.7935 (2) | 0.85284 (7) | 0.0255 (3) |
| C25 | 0.00430 (9)  | 0.7460 (3) | 0.91150 (7) | 0.0302 (3) |
| H25 | 0.0134       | 0.8432     | 0.9572      | 0.036*     |
| C26 | 0.06596 (9)  | 0.5553 (3) | 0.90256 (7) | 0.0299 (3) |
| H26 | 0.1179       | 0.5209     | 0.9420      | 0.036*     |

### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|------------|------------|------------|-------------|-------------|-------------|
| N1  | 0.0236 (5) | 0.0169 (5) | 0.0340 (6) | 0.0039 (4)  | 0.0074 (4)  | 0.0037 (4)  |
| N2  | 0.0215 (5) | 0.0311 (6) | 0.0381 (6) | -0.0002 (4) | 0.0029 (5)  | -0.0022 (5) |
| O1  | 0.0261 (5) | 0.0180 (4) | 0.0503 (6) | 0.0026 (4)  | 0.0045 (4)  | 0.0018 (4)  |
| O2  | 0.0229 (5) | 0.0270 (5) | 0.0462 (6) | -0.0025 (4) | 0.0065 (4)  | -0.0104 (4) |
| O3  | 0.0393 (6) | 0.0555 (7) | 0.0490 (7) | 0.0155 (5)  | -0.0018 (5) | -0.0224 (6) |
| O4  | 0.0289 (5) | 0.0452 (6) | 0.0466 (6) | 0.0089 (4)  | -0.0032 (4) | 0.0036 (5)  |
| C1  | 0.0237 (6) | 0.0209 (6) | 0.0264 (6) | 0.0024 (5)  | 0.0068 (5)  | 0.0025 (5)  |
| C2  | 0.0255 (6) | 0.0230 (6) | 0.0387 (7) | 0.0032 (5)  | 0.0070 (5)  | 0.0058 (5)  |
| C3  | 0.0265 (7) | 0.0322 (7) | 0.0493 (8) | 0.0022 (6)  | 0.0133 (6)  | 0.0065 (6)  |
| C11 | 0.0240 (6) | 0.0196 (5) | 0.0253 (6) | 0.0015 (4)  | 0.0078 (5)  | -0.0020 (4) |
| C12 | 0.0291 (7) | 0.0210 (6) | 0.0382 (7) | 0.0034 (5)  | 0.0090 (5)  | 0.0068 (5)  |
| C13 | 0.0297 (7) | 0.0218 (6) | 0.0418 (7) | -0.0017 (5) | 0.0136 (6)  | 0.0038 (5)  |
| C14 | 0.0222 (6) | 0.0234 (6) | 0.0303 (6) | -0.0001 (5) | 0.0073 (5)  | -0.0063 (5) |
| C15 | 0.0269 (6) | 0.0237 (6) | 0.0292 (6) | 0.0023 (5)  | 0.0030 (5)  | 0.0030 (5)  |
| C16 | 0.0262 (6) | 0.0231 (6) | 0.0283 (6) | -0.0016 (5) | 0.0062 (5)  | 0.0040 (5)  |
| C21 | 0.0204 (6) | 0.0243 (6) | 0.0317 (7) | -0.0026 (5) | 0.0082 (5)  | -0.0015 (5) |
| C22 | 0.0286 (7) | 0.0361 (7) | 0.0269 (6) | -0.0046 (5) | 0.0033 (5)  | -0.0081 (5) |
| C23 | 0.0228 (6) | 0.0382 (7) | 0.0277 (7) | -0.0020 (5) | -0.0018 (5) | -0.0015 (5) |
| C24 | 0.0188 (6) | 0.0273 (6) | 0.0306 (6) | -0.0013 (5) | 0.0055 (5)  | -0.0002 (5) |
| C25 | 0.0260 (6) | 0.0372 (7) | 0.0260 (6) | 0.0020 (5)  | 0.0018 (5)  | -0.0077 (6) |
| C26 | 0.0231 (6) | 0.0365 (7) | 0.0275 (7) | 0.0029 (5)  | -0.0007 (5) | -0.0024 (5) |

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

|        |             |         |             |
|--------|-------------|---------|-------------|
| N1—C1  | 1.3613 (16) | C12—C13 | 1.3954 (19) |
| N1—C11 | 1.4270 (16) | C12—H12 | 0.9500      |
| N1—H1  | 0.825 (17)  | C13—C14 | 1.3849 (18) |
| N2—O4  | 1.2273 (15) | C13—H13 | 0.9500      |
| N2—O3  | 1.2314 (15) | C14—C15 | 1.3910 (18) |
| N2—C24 | 1.4678 (16) | C15—C16 | 1.3976 (18) |
| O1—C1  | 1.2339 (15) | C15—H15 | 0.9500      |
| O2—C21 | 1.3842 (15) | C16—H16 | 0.9500      |
| O2—C14 | 1.4047 (15) | C21—C26 | 1.3899 (18) |
| C1—C2  | 1.5233 (17) | C21—C22 | 1.3938 (18) |
| C2—C3  | 1.5201 (18) | C22—C23 | 1.389 (2)   |
| C2—H2A | 0.9900      | C22—H22 | 0.9500      |
| C2—H2B | 0.9900      | C23—C24 | 1.3875 (18) |
| C3—H3A | 0.9800      | C23—H23 | 0.9500      |

|                 |              |                 |              |
|-----------------|--------------|-----------------|--------------|
| C3—H3B          | 0.9800       | C24—C25         | 1.3894 (18)  |
| C3—H3C          | 0.9800       | C25—C26         | 1.3871 (18)  |
| C11—C12         | 1.3965 (17)  | C25—H25         | 0.9500       |
| C11—C16         | 1.3972 (17)  | C26—H26         | 0.9500       |
| C1—N1—C11       | 126.93 (10)  | C14—C13—H13     | 120.4        |
| C1—N1—H1        | 117.5 (11)   | C12—C13—H13     | 120.4        |
| C11—N1—H1       | 115.4 (11)   | C13—C14—C15     | 120.99 (11)  |
| O4—N2—O3        | 122.86 (12)  | C13—C14—O2      | 118.22 (11)  |
| O4—N2—C24       | 118.75 (11)  | C15—C14—O2      | 120.49 (11)  |
| O3—N2—C24       | 118.38 (11)  | C14—C15—C16     | 119.71 (11)  |
| C21—O2—C14      | 117.81 (9)   | C14—C15—H15     | 120.1        |
| O1—C1—N1        | 123.01 (11)  | C16—C15—H15     | 120.1        |
| O1—C1—C2        | 121.87 (11)  | C11—C16—C15     | 119.90 (11)  |
| N1—C1—C2        | 115.10 (10)  | C11—C16—H16     | 120.0        |
| C3—C2—C1        | 112.62 (10)  | C15—C16—H16     | 120.0        |
| C3—C2—H2A       | 109.1        | O2—C21—C26      | 121.72 (11)  |
| C1—C2—H2A       | 109.1        | O2—C21—C22      | 116.88 (11)  |
| C3—C2—H2B       | 109.1        | C26—C21—C22     | 121.31 (12)  |
| C1—C2—H2B       | 109.1        | C23—C22—C21     | 119.47 (12)  |
| H2A—C2—H2B      | 107.8        | C23—C22—H22     | 120.3        |
| C2—C3—H3A       | 109.5        | C21—C22—H22     | 120.3        |
| C2—C3—H3B       | 109.5        | C24—C23—C22     | 118.89 (12)  |
| H3A—C3—H3B      | 109.5        | C24—C23—H23     | 120.6        |
| C2—C3—H3C       | 109.5        | C22—C23—H23     | 120.6        |
| H3A—C3—H3C      | 109.5        | C23—C24—C25     | 121.81 (12)  |
| H3B—C3—H3C      | 109.5        | C23—C24—N2      | 119.11 (11)  |
| C12—C11—C16     | 119.52 (11)  | C25—C24—N2      | 119.08 (11)  |
| C12—C11—N1      | 117.63 (11)  | C26—C25—C24     | 119.30 (12)  |
| C16—C11—N1      | 122.80 (11)  | C26—C25—H25     | 120.4        |
| C13—C12—C11     | 120.68 (12)  | C24—C25—H25     | 120.4        |
| C13—C12—H12     | 119.7        | C25—C26—C21     | 119.22 (12)  |
| C11—C12—H12     | 119.7        | C25—C26—H26     | 120.4        |
| C14—C13—C12     | 119.20 (11)  | C21—C26—H26     | 120.4        |
| C11—N1—C1—O1    | -2.4 (2)     | C14—C15—C16—C11 | -0.06 (19)   |
| C11—N1—C1—C2    | 176.22 (11)  | C14—O2—C21—C26  | -43.11 (17)  |
| O1—C1—C2—C3     | -34.15 (18)  | C14—O2—C21—C22  | 140.29 (12)  |
| N1—C1—C2—C3     | 147.24 (12)  | O2—C21—C22—C23  | 177.11 (11)  |
| C1—N1—C11—C12   | -148.08 (13) | C26—C21—C22—C23 | 0.5 (2)      |
| C1—N1—C11—C16   | 34.49 (19)   | C21—C22—C23—C24 | 0.0 (2)      |
| C16—C11—C12—C13 | 0.35 (19)    | C22—C23—C24—C25 | -0.6 (2)     |
| N1—C11—C12—C13  | -177.16 (12) | C22—C23—C24—N2  | 179.81 (12)  |
| C11—C12—C13—C14 | 0.4 (2)      | O4—N2—C24—C23   | -6.26 (18)   |
| C12—C13—C14—C15 | -1.02 (19)   | O3—N2—C24—C23   | 172.74 (13)  |
| C12—C13—C14—O2  | 172.67 (11)  | O4—N2—C24—C25   | 174.14 (12)  |
| C21—O2—C14—C13  | 129.12 (12)  | O3—N2—C24—C25   | -6.86 (18)   |
| C21—O2—C14—C15  | -57.16 (16)  | C23—C24—C25—C26 | 0.8 (2)      |
| C13—C14—C15—C16 | 0.85 (19)    | N2—C24—C25—C26  | -179.65 (12) |
| O2—C14—C15—C16  | -172.70 (11) | C24—C25—C26—C21 | -0.3 (2)     |

## supplementary materials

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|                 |             |                 |              |
|-----------------|-------------|-----------------|--------------|
| C12—C11—C16—C15 | -0.53 (18)  | O2—C21—C26—C25  | -176.78 (12) |
| N1—C11—C16—C15  | 176.85 (11) | C22—C21—C26—C25 | -0.3 (2)     |

### Hydrogen-bond geometry (Å, °)

| <i>D</i> —H $\cdots$ <i>A</i>      | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N1—H1 $\cdots$ O1 <sup>i</sup>     | 0.825 (17)  | 2.255 (17)          | 3.0306 (13)                | 156.7 (15)                    |
| C25—H25 $\cdots$ O3 <sup>ii</sup>  | 0.95        | 2.42                | 3.2082 (17)                | 140                           |
| C23—H23 $\cdots$ O4 <sup>iii</sup> | 0.95        | 2.53                | 3.3400 (16)                | 144                           |

Symmetry codes: (i)  $x, y-1, z$ ; (ii)  $-x, -y+2, -z+2$ ; (iii)  $-x-1/2, y-1/2, -z+3/2$ .



Fig. 1

