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# 2-[2-(1,3-Dioxoisoindolin-2-yl)phenyl]-isoindoline-1,3-dione

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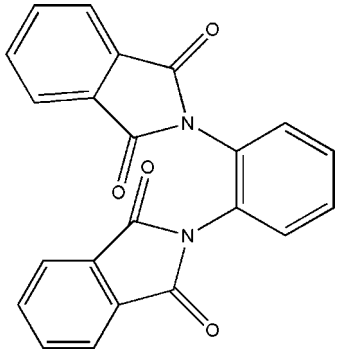
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.041; $wR$ factor = 0.094; data-to-parameter ratio = 13.7.

In the title compound, $C_{22}H_{12}N_2O_4$, the two isoindolinyl groups are twisted with respect to the benzene ring, with dihedral angles of 58.15 (7) and 61.32 (7)°; the dihedral angle between the two isoindolinyl groups is 39.45 (6)°. The molecules are linked together by weak C—H···O hydrogen bonding.

## Related literature

For general background, see: Pendrak *et al.* (1994); De Clerck (1995); Stowers (1996); Heaney & Shuhaibar (1995). For a related structure, see: Liang & Li (2007).



## Experimental

### Crystal data

$C_{22}H_{12}N_2O_4$
$M_r$ = 368.34
Monoclinic, $P2_1/n$
$a$ = 10.7765 (10) Å
$b$ = 16.9259 (17) Å
$c$ = 10.8518 (10) Å
$\beta$ = 116.780 (1)°
$V$ = 1767.1 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 293 (2) K
0.35 × 0.33 × 0.28 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
9771 measured reflections
3476 independent reflections
2553 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.050

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.094
$S$ = 0.95
3476 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C13—H13$A$···O4$^{i}$ | 0.93 | 2.39 | 3.321 (2) | 179 |
| C24—H24$A$···O3$^{ii}$ | 0.93 | 2.51 | 3.405 (2) | 161 |
| C26—H26$A$···O1$^{iii}$ | 0.93 | 2.53 | 3.434 (2) | 164 |
| C34—H34$A$···O2$^{iv}$ | 0.93 | 2.48 | 3.410 (2) | 177 |
| C36—H36$A$···O2$^{v}$ | 0.93 | 2.55 | 3.255 (2) | 133 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2298).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o3694 [ **doi:10.1107/S1600536807037038** ]

# 2-[2-(1,3-Dioxoisoindolin-2-yl)phenyl]isoindoline-1,3-dione

**X.-Y. Wu, D.-S. Zhu, Y.-H. Wang and C.-G. Zhu**

## Comment

Isoindolinones and their derivatives have been investigated widely due to their profound physiological and chemotherapeutic properties. Many compounds containing the isoindolinone skeleton have shown antiviral, antileukemic, antiinflammatory, antipsychotic and antiulcer properties (Pendrak *et al.*, 1994; De Clerck, 1995). Isoindolinones are useful for the synthesis of various drugs and naturally occurring compounds (Stowers, 1996; Heaney & Shuhaibar, 1995). In this paper, we report the crystal structure of the title compound.

As shown in Fig. 1, the structure determination indicates that the molecule is non-centrosymmetric. Due to steric encumbering, two isoindolinyl moieties are twisted to the benzene ring with dihedral angles of 58.15 (7) and 61.32 (7)°, respectively, similar to 62.31 (6)° found in 2-(2-pyridyl)isoindoline-1,3-dione (Liang & Li, 2007). The dihedral angle between the two isoindolinyl moieties is 39.45 (6)°. The molecules are linked together by weak C—H···O hydrogen bonding (Table 1).

## Experimental

*O*-Phenylenediamine (0.11 g, 1 mmol) was dissolved in 5 ml glacial acetic acid, and a solution of phthalic anhydride (0.148 g, 1 mmol) in 10 ml of glacial acetic acid was added. After 30 min, the mixture was diluted with cool water, and then the grey precipitate was separated and then refluxed in dry benzene (20 ml) for 4 h using Dean and Stark apparatus. After solvent was removed under reduced pressure the solid product was obtained. The colorless single crystals of the title compound were obtained by recrystallization from an ethanol solution at room temperature after 2 d.

## Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Figures

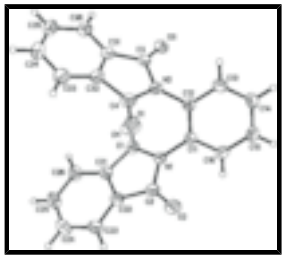


Fig. 1. A view of the molecule of (I). Displacement ellipsoids are drawn at the 50% probability level.

### 2-[2-(1,3-Dioxoisoindolin-2-yl)phenyl]isoindoline-1,3-dione

*Crystal data*

| | |
|---|---|
| $C_{22}H_{12}N_2O_4$ | $F_{000}$ = 760 |
| $M_r$ = 368.34 | $D_x$ = 1.385 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>$\lambda$ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 9771 reflections |
| $a$ = 10.7765 (10) Å | $\theta$ = 2.2–26.0º |
| $b$ = 16.9259 (17) Å | $\mu$ = 0.10 mm$^{-1}$ |
| $c$ = 10.8518 (10) Å | $T$ = 293 (2) K |
| $\beta$ = 116.780 (1)º | Block, colourless |
| $V$ = 1767.1 (3) Å$^3$ | 0.35 × 0.33 × 0.28 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2553 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.050 |
| Monochromator: graphite | $\theta_{max}$ = 26.0º |
| $T$ = 293(2) K | $\theta_{min}$ = 2.2º |
| $\varphi$ and $\omega$ scans | $h$ = −9→13 |
| Absorption correction: none | $k$ = −16→20 |
| 9771 measured reflections | $l$ = −13→13 |
| 3476 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 |
| $R[F^2 > 2\sigma(F^2)]$ = 0.041 | H-atom parameters constrained |
| $wR(F^2)$ = 0.094 | $w = 1/[\sigma^2(F_o^2) + (0.0421P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.95 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 3476 reflections | $\Delta\rho_{max}$ = 0.20 e Å$^{-3}$ |
| 253 parameters | $\Delta\rho_{min}$ = −0.19 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | 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.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on $F^2$, conventional *R*-factors *R* are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and *R*-factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.45581 (11) | 0.01749 (7) | 0.14315 (11) | 0.0365 (3) |
| O2 | 0.07744 (11) | 0.13152 (8) | 0.15937 (12) | 0.0437 (4) |
| O3 | 0.74820 (11) | 0.10013 (7) | 0.38688 (11) | 0.0322 (3) |
| O4 | 0.34849 (12) | 0.24241 (7) | 0.14859 (13) | 0.0411 (3) |
| N1 | 0.28632 (13) | 0.07596 (8) | 0.18964 (12) | 0.0264 (3) |
| N2 | 0.53713 (12) | 0.16715 (8) | 0.29363 (13) | 0.0257 (3) |
| C1 | 0.34000 (17) | 0.04363 (10) | 0.10366 (16) | 0.0277 (4) |
| C2 | 0.14769 (16) | 0.10141 (10) | 0.11178 (16) | 0.0296 (4) |
| C3 | 0.66539 (16) | 0.14316 (10) | 0.29978 (16) | 0.0252 (4) |
| C4 | 0.46318 (17) | 0.21605 (10) | 0.17971 (16) | 0.0296 (4) |
| C11 | 0.36534 (16) | 0.09109 (10) | 0.33430 (15) | 0.0250 (4) |
| C12 | 0.48509 (16) | 0.13677 (10) | 0.38461 (16) | 0.0251 (4) |
| C13 | 0.55851 (17) | 0.15123 (10) | 0.52504 (16) | 0.0312 (4) |
| H13A | 0.6389 | 0.1817 | 0.5587 | 0.037* |
| C14 | 0.51259 (18) | 0.12054 (11) | 0.61507 (17) | 0.0339 (4) |
| H14A | 0.5619 | 0.1304 | 0.7092 | 0.041* |
| C15 | 0.39354 (18) | 0.07529 (11) | 0.56535 (16) | 0.0336 (4) |
| H15A | 0.3629 | 0.0544 | 0.6261 | 0.040* |
| C16 | 0.31966 (17) | 0.06088 (10) | 0.42531 (16) | 0.0301 (4) |
| H16A | 0.2389 | 0.0307 | 0.3921 | 0.036* |
| C21 | 0.22647 (16) | 0.05014 (10) | −0.03928 (15) | 0.0268 (4) |
| C22 | 0.11188 (16) | 0.08397 (10) | −0.03443 (16) | 0.0283 (4) |
| C23 | −0.00825 (18) | 0.09885 (11) | −0.15363 (17) | 0.0352 (4) |
| H23A | −0.0856 | 0.1211 | −0.1505 | 0.042* |
| C24 | −0.00952 (18) | 0.07944 (11) | −0.27824 (17) | 0.0374 (4) |
| H24A | −0.0890 | 0.0892 | −0.3602 | 0.045* |
| C25 | 0.10523 (18) | 0.04581 (11) | −0.28296 (17) | 0.0388 (5) |
| H25A | 0.1015 | 0.0332 | −0.3680 | 0.047* |
| C26 | 0.22624 (18) | 0.03050 (11) | −0.16251 (16) | 0.0347 (4) |
| H26A | 0.3037 | 0.0079 | −0.1652 | 0.042* |
| C31 | 0.67265 (16) | 0.18160 (10) | 0.18068 (15) | 0.0270 (4) |
| C32 | 0.55298 (16) | 0.22536 (10) | 0.10967 (16) | 0.0295 (4) |
| C33 | 0.53101 (18) | 0.26772 (11) | −0.00715 (18) | 0.0392 (5) |
| H33A | 0.4505 | 0.2973 | −0.0546 | 0.047* |
| C34 | 0.63355 (19) | 0.26451 (12) | −0.05105 (18) | 0.0429 (5) |
| H34A | 0.6214 | 0.2921 | −0.1298 | 0.051* |
| C35 | 0.75357 (19) | 0.22099 (11) | 0.02044 (18) | 0.0388 (5) |
| H35A | 0.8211 | 0.2203 | −0.0107 | 0.047* |

| | | | | |
|---|---|---|---|---|
| C36 | 0.77526 (17) | 0.17830 (11) | 0.13755 (17) | 0.0327 (4) |
| H36A | 0.8556 | 0.1487 | 0.1851 | 0.039* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0277 (7) | 0.0500 (8) | 0.0315 (6) | 0.0109 (6) | 0.0132 (5) | −0.0002 (6) |
| O2 | 0.0273 (7) | 0.0680 (10) | 0.0370 (7) | 0.0069 (6) | 0.0156 (6) | −0.0122 (6) |
| O3 | 0.0240 (6) | 0.0402 (8) | 0.0282 (6) | 0.0050 (6) | 0.0082 (5) | 0.0051 (5) |
| O4 | 0.0267 (7) | 0.0422 (8) | 0.0558 (8) | 0.0104 (6) | 0.0199 (6) | 0.0156 (6) |
| N1 | 0.0210 (7) | 0.0358 (8) | 0.0233 (7) | 0.0002 (6) | 0.0107 (6) | −0.0034 (6) |
| N2 | 0.0197 (7) | 0.0312 (8) | 0.0268 (7) | 0.0019 (6) | 0.0112 (6) | 0.0054 (6) |
| C1 | 0.0277 (9) | 0.0297 (10) | 0.0280 (9) | 0.0000 (8) | 0.0145 (8) | −0.0010 (7) |
| C2 | 0.0228 (9) | 0.0361 (11) | 0.0305 (9) | −0.0017 (8) | 0.0124 (8) | −0.0034 (8) |
| C3 | 0.0198 (8) | 0.0288 (10) | 0.0254 (8) | −0.0027 (7) | 0.0087 (7) | −0.0018 (7) |
| C4 | 0.0247 (9) | 0.0293 (10) | 0.0339 (9) | 0.0008 (8) | 0.0123 (8) | 0.0039 (8) |
| C11 | 0.0224 (9) | 0.0304 (10) | 0.0223 (8) | 0.0031 (7) | 0.0101 (7) | −0.0011 (7) |
| C12 | 0.0225 (8) | 0.0281 (9) | 0.0260 (8) | 0.0024 (7) | 0.0122 (7) | 0.0019 (7) |
| C13 | 0.0247 (9) | 0.0353 (11) | 0.0299 (9) | −0.0026 (8) | 0.0090 (8) | −0.0035 (8) |
| C14 | 0.0342 (10) | 0.0432 (12) | 0.0220 (8) | 0.0019 (9) | 0.0107 (8) | −0.0014 (8) |
| C15 | 0.0367 (10) | 0.0413 (11) | 0.0286 (9) | 0.0010 (9) | 0.0197 (8) | 0.0039 (8) |
| C16 | 0.0267 (9) | 0.0343 (11) | 0.0331 (9) | −0.0029 (8) | 0.0168 (8) | −0.0006 (8) |
| C21 | 0.0251 (9) | 0.0294 (10) | 0.0252 (8) | 0.0009 (7) | 0.0108 (7) | −0.0002 (7) |
| C22 | 0.0244 (9) | 0.0328 (10) | 0.0273 (9) | −0.0019 (8) | 0.0113 (7) | −0.0035 (7) |
| C23 | 0.0247 (9) | 0.0423 (12) | 0.0329 (9) | 0.0027 (8) | 0.0080 (8) | −0.0035 (8) |
| C24 | 0.0338 (10) | 0.0401 (11) | 0.0276 (9) | 0.0002 (9) | 0.0043 (8) | 0.0007 (8) |
| C25 | 0.0441 (11) | 0.0454 (12) | 0.0243 (9) | 0.0004 (9) | 0.0131 (9) | −0.0043 (8) |
| C26 | 0.0366 (10) | 0.0402 (11) | 0.0294 (9) | 0.0046 (9) | 0.0167 (8) | −0.0024 (8) |
| C31 | 0.0240 (9) | 0.0300 (10) | 0.0271 (8) | −0.0024 (7) | 0.0117 (7) | −0.0002 (7) |
| C32 | 0.0245 (9) | 0.0335 (10) | 0.0309 (9) | −0.0004 (8) | 0.0127 (8) | 0.0041 (8) |
| C33 | 0.0325 (10) | 0.0434 (12) | 0.0395 (10) | 0.0044 (9) | 0.0143 (9) | 0.0137 (9) |
| C34 | 0.0461 (12) | 0.0509 (13) | 0.0350 (10) | −0.0047 (10) | 0.0214 (9) | 0.0104 (9) |
| C35 | 0.0397 (11) | 0.0485 (13) | 0.0373 (10) | −0.0071 (9) | 0.0253 (9) | −0.0013 (9) |
| C36 | 0.0278 (9) | 0.0378 (11) | 0.0340 (9) | −0.0005 (8) | 0.0152 (8) | −0.0010 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.2063 (18) | C15—H15A | 0.9300 |
| O2—C2 | 1.2050 (18) | C16—H16A | 0.9300 |
| O3—C3 | 1.2083 (18) | C21—C26 | 1.377 (2) |
| O4—C4 | 1.2101 (18) | C21—C22 | 1.384 (2) |
| N1—C1 | 1.4110 (19) | C22—C23 | 1.380 (2) |
| N1—C2 | 1.412 (2) | C23—C24 | 1.386 (2) |
| N1—C11 | 1.4320 (18) | C23—H23A | 0.9300 |
| N2—C4 | 1.400 (2) | C24—C25 | 1.383 (2) |
| N2—C3 | 1.4131 (19) | C24—H24A | 0.9300 |
| N2—C12 | 1.4328 (19) | C25—C26 | 1.393 (2) |
| C1—C21 | 1.485 (2) | C25—H25A | 0.9300 |
| C2—C22 | 1.484 (2) | C26—H26A | 0.9300 |

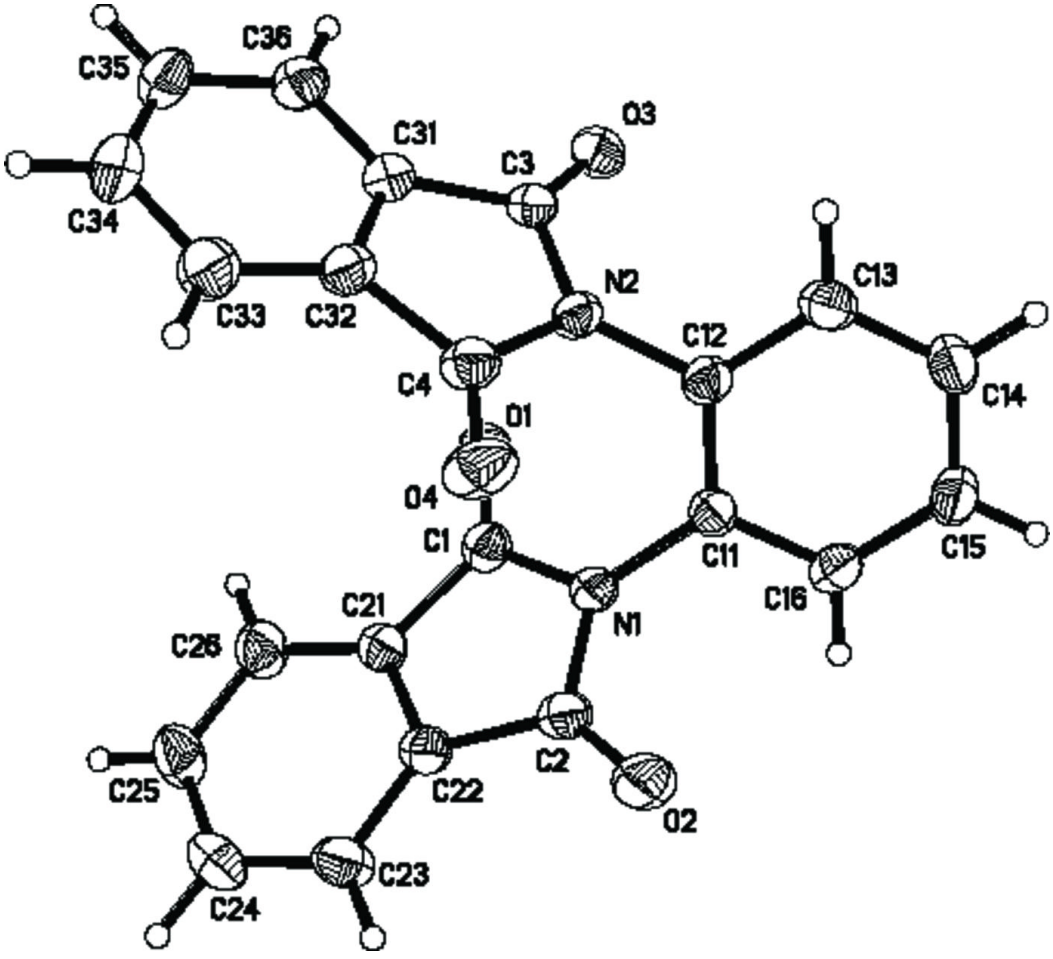
| | | | |
|---|---|---|---|
| C3—C31 | 1.480 (2) | C31—C32 | 1.382 (2) |
| C4—C32 | 1.484 (2) | C31—C36 | 1.383 (2) |
| C11—C16 | 1.385 (2) | C32—C33 | 1.381 (2) |
| C11—C12 | 1.388 (2) | C33—C34 | 1.388 (2) |
| C12—C13 | 1.386 (2) | C33—H33A | 0.9300 |
| C13—C14 | 1.380 (2) | C34—C35 | 1.383 (2) |
| C13—H13A | 0.9300 | C34—H34A | 0.9300 |
| C14—C15 | 1.378 (2) | C35—C36 | 1.387 (2) |
| C14—H14A | 0.9300 | C35—H35A | 0.9300 |
| C15—C16 | 1.383 (2) | C36—H36A | 0.9300 |
| C1—N1—C2 | 111.16 (13) | C26—C21—C22 | 121.72 (15) |
| C1—N1—C11 | 125.16 (13) | C26—C21—C1 | 129.55 (15) |
| C2—N1—C11 | 123.21 (12) | C22—C21—C1 | 108.68 (13) |
| C4—N2—C3 | 111.54 (12) | C23—C22—C21 | 121.09 (15) |
| C4—N2—C12 | 125.22 (12) | C23—C22—C2 | 130.42 (15) |
| C3—N2—C12 | 122.86 (13) | C21—C22—C2 | 108.45 (14) |
| O1—C1—N1 | 125.04 (14) | C22—C23—C24 | 117.67 (16) |
| O1—C1—C21 | 129.19 (15) | C22—C23—H23A | 121.2 |
| N1—C1—C21 | 105.77 (13) | C24—C23—H23A | 121.2 |
| O2—C2—N1 | 124.91 (15) | C25—C24—C23 | 121.19 (16) |
| O2—C2—C22 | 129.15 (15) | C25—C24—H24A | 119.4 |
| N1—C2—C22 | 105.93 (13) | C23—C24—H24A | 119.4 |
| O3—C3—N2 | 124.90 (14) | C24—C25—C26 | 121.09 (16) |
| O3—C3—C31 | 129.57 (14) | C24—C25—H25A | 119.5 |
| N2—C3—C31 | 105.53 (13) | C26—C25—H25A | 119.5 |
| O4—C4—N2 | 124.59 (15) | C21—C26—C25 | 117.24 (16) |
| O4—C4—C32 | 129.63 (15) | C21—C26—H26A | 121.4 |
| N2—C4—C32 | 105.77 (13) | C25—C26—H26A | 121.4 |
| C16—C11—C12 | 119.44 (14) | C32—C31—C36 | 121.38 (15) |
| C16—C11—N1 | 119.27 (14) | C32—C31—C3 | 108.62 (13) |
| C12—C11—N1 | 121.28 (13) | C36—C31—C3 | 130.00 (15) |
| C13—C12—C11 | 119.99 (14) | C33—C32—C31 | 121.41 (15) |
| C13—C12—N2 | 119.17 (14) | C33—C32—C4 | 130.07 (15) |
| C11—C12—N2 | 120.81 (13) | C31—C32—C4 | 108.52 (14) |
| C14—C13—C12 | 120.17 (15) | C32—C33—C34 | 117.47 (16) |
| C14—C13—H13A | 119.9 | C32—C33—H33A | 121.3 |
| C12—C13—H13A | 119.9 | C34—C33—H33A | 121.3 |
| C15—C14—C13 | 119.96 (15) | C35—C34—C33 | 121.09 (16) |
| C15—C14—H14A | 120.0 | C35—C34—H34A | 119.5 |
| C13—C14—H14A | 120.0 | C33—C34—H34A | 119.5 |
| C14—C15—C16 | 120.11 (15) | C34—C35—C36 | 121.35 (16) |
| C14—C15—H15A | 119.9 | C34—C35—H35A | 119.3 |
| C16—C15—H15A | 119.9 | C36—C35—H35A | 119.3 |
| C15—C16—C11 | 120.33 (15) | C31—C36—C35 | 117.31 (16) |
| C15—C16—H16A | 119.8 | C31—C36—H36A | 121.3 |
| C11—C16—H16A | 119.8 | C35—C36—H36A | 121.3 |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13A···O4$^{i}$ | 0.93 | 2.39 | 3.321 (2) | 179 |
| C24—H24A···O3$^{ii}$ | 0.93 | 2.51 | 3.405 (2) | 161 |
| C26—H26A···O1$^{iii}$ | 0.93 | 2.53 | 3.434 (2) | 164 |
| C34—H34A···O2$^{iv}$ | 0.93 | 2.48 | 3.410 (2) | 177 |
| C36—H36A···O2$^{v}$ | 0.93 | 2.55 | 3.255 (2) | 133 |

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

Fig. 1


C36
C35
C31
O3
C3
C34
N2
C13
C33
C32
C12
C4
C14
O1
O4
C1
C11
C15
C21
N1
C16
C26
C2
C25
C22
O2
C23
C24