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# 3-(2-Hydroxyphenyl)-5-(2-methoxyphenyl)-1*H*-pyrazole

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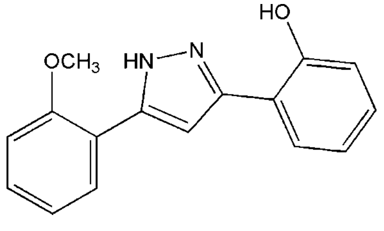
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.035; $wR$ factor = 0.091; data-to-parameter ratio = 9.3.

The title compound, $C_{16}H_{14}N_2O_2$, was derived from 1-(2-hydroxyphenyl)-3-(2-methoxyphenyl)propane-1,3-dione. The molecule is essentially planar (r.m.s. deviation for all non-H atoms = 0.089 Å). Two intramolecular hydrogen bonds stabilize the molecular conformation and one N—H···O hydrogen bond stabilizes the crystal structure.

## Related literature

For related literature, see: Ahmad *et al.* (1990, 1997); Ezava *et al.* (2005); Feierman & Cederbaum (1986); Sanz *et al.* (1998); Alcaraz *et al.* (1993); Hamper *et al.* (1997); Fujio (1999).




## Experimental

*Crystal data*

$C_{16}H_{14}N_2O_2$
$M_r$ = 266.29
Orthorhombic, $Pna2_1$
$a$ = 17.5626 (15) Å
$b$ = 10.2239 (7) Å
$c$ = 7.4513 (7) Å
$V$ = 1337.94 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 173 (2) K
0.27 × 0.25 × 0.24 mm

*Data collection*

Stoe IPDSII two-circle diffractometer
Absorption correction: none
10969 measured reflections
1777 independent reflections
1620 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.090
$S$ = 1.03
1777 reflections
191 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2···N2 | 0.99 (4) | 1.64 (4) | 2.560 (2) | 152 (3) |
| N1—H1···O1 | 0.92 (3) | 2.07 (3) | 2.628 (2) | 118 (2) |
| N1—H1···O2$^{i}$ | 0.92 (3) | 2.09 (3) | 2.892 (2) | 146 (3) |

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; 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: BX2163).

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# supplementary materials

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## 3-(2-Hydroxyphenyl)-5-(2-methoxyphenyl)-1*H*-pyrazole

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### Comment

3,5-substituted Pyrazoles are important class of compounds.These have been proven to be a selective inhibitor of COX in isoenzyme in human blood and are used for the development of anti-inflamatory drugs and analgesic medicines (Ezava *et al.*, 2005). Disubstituted pyrazoles have been reported as an important intermediate in the synthesis of herbicides (US patent 5191087, 1993; US patent 5698708, 1997) and for the treatmet of pain and disorders such as Arthritis (US patent 5908857, 1999).Pyrazoles are inhibitors of alchol dehydrogenase and have been found to be effective inhibitors for the oxidation of ethanol by liver microsomes (Feierman & Cederbaum, 1986). 3,5-disubstituted pyrazoles are also uesd to form solid dinuclear complexes (Sanz *et al.*, 1998). The molecule is essentially planar (r.m.s. deviation for all non-H atoms 0.089 Å). Two intramolecular hydrogen bonds stabilize the molecular conformation and one N—H···O hydrogen bond is stabilizing the crystal structure.

### Experimental

1-(2'-hydroxyphenyl)-3-(2''-methoxyphenyl) propane-1,3-dione was prepared by a modified Baker Venkataram rearrangement as reported earlier (Ahmad *et al.*, 1997). Purification was carried out by recrystallization using absolute ethanol. 1-*H*-3(2-hydroxyphenyl)-5-(2-methoxyphenyl) pyrazole was synthesized by reacting hydrazine hydrate (0.5 g, 10 mmol) with 1-(2-hydroxyphenyl)-3-(2-methoxyphenyl) propane-1,3-dione (2.7 g, 10 mmol) in 100 ml of absolute ethanol. The mixture was refluxed for seven hours. Solvent was removed under reduced pressure. Compound (II) was synthesized by adding 0.1 mole of phenyl hydrazine in 0.1 mole of compound (II) dissolved in 200 ml of absolute ethanol. The mixture was refluxed for 7 h. Solvent was removed under reduced pressure. Highly viscous residue was recrystallized using absolute ethanol. (Yield: 96%, m.p: 456k)

### Refinement

In the absence of anomalous scatterers 1544 Friedel pairs were merged. H atoms were located in a difference map, but those bonded to C were geometrically positioned and refined using a riding model with fixed individual displacement parameters [$U(H) = 1.2\ U_{eq}(C)$ or $U(H) = 1.5\ U_{eq}(C_{methyl})$] and with C—H = 0.95 Å or $C_{methyl}$—H = 0.98 Å. The methyl group was allowed to rotate but not to tip. The H atoms bonded to N and O were freely refined.

### Figures

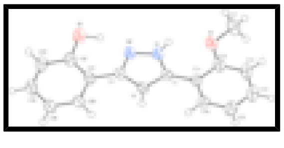


Fig. 1. Perspective view of the title compound with the atom numbering scheme; displacement ellipsoids are at the 50% probability level; H atoms are drawn as small spheres of arbitrary radii.

## 3-(2-Hydroxyphenyl)-5-(2-methoxyphenyl)-1H-pyrazole

### *Crystal data*

| | |
|---|---|
| $C_{16}H_{14}N_2O_2$ | $D_x$ = 1.322 Mg m$^{-3}$ |
| $M_r$ = 266.29 | Melting point: 456 K |
| Orthorhombic, $Pna2_1$ | Mo $K\alpha$ radiation<br>$\lambda$ = 0.71073 Å |
| Hall symbol: P 2c -2n | Cell parameters from 11915 reflections |
| $a$ = 17.5626 (15) Å | $\theta$ = 3.4–29.6° |
| $b$ = 10.2239 (7) Å | $\mu$ = 0.09 mm$^{-1}$ |
| $c$ = 7.4513 (7) Å | $T$ = 173 (2) K |
| $V$ = 1337.94 (19) Å$^3$ | Block, light yellow |
| $Z$ = 4 | 0.27 × 0.25 × 0.24 mm |
| $F_{000}$ = 560 | |

### *Data collection*

| | |
|---|---|
| Stoe IPDSII two-circle diffractometer | 1620 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.057 |
| Monochromator: graphite | $\theta_{max}$ = 28.3° |
| $T$ = 173(2) K | $\theta_{min}$ = 3.6° |
| ω scans | $h$ = −20→23 |
| Absorption correction: none | $k$ = −11→13 |
| 10969 measured reflections | $l$ = −8→9 |
| 1777 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 |
| $R[F^2 > 2\sigma(F^2)]$ = 0.034 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.091 | $w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.0395P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.03 | $(\Delta/\sigma)_{max}$ < 0.001 |
| 1777 reflections | $\Delta\rho_{max}$ = 0.18 e Å$^{-3}$ |
| 191 parameters | $\Delta\rho_{min}$ = −0.16 e Å$^{-3}$ |
| 1 restraint | Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.049 (6) |

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.49830 (7) | 0.72482 (13) | 0.76358 (19) | 0.0401 (3) |
| O2 | 0.42612 (9) | 1.04511 (15) | 0.0584 (2) | 0.0507 (4) |
| H2 | 0.441 (2) | 0.992 (4) | 0.165 (6) | 0.093 (11)* |
| N1 | 0.44362 (8) | 0.80017 (15) | 0.4520 (2) | 0.0340 (3) |
| H1 | 0.4833 (15) | 0.825 (3) | 0.525 (4) | 0.058 (7)* |
| N2 | 0.43083 (8) | 0.86611 (15) | 0.2984 (2) | 0.0369 (3) |
| C1 | 0.39489 (9) | 0.69783 (15) | 0.4736 (2) | 0.0289 (3) |
| C2 | 0.34823 (9) | 0.69776 (15) | 0.3232 (2) | 0.0306 (3) |
| H2A | 0.3083 | 0.6381 | 0.2968 | 0.037* |
| C3 | 0.37225 (9) | 0.80434 (16) | 0.2179 (2) | 0.0304 (3) |
| C11 | 0.39509 (9) | 0.61110 (16) | 0.6314 (2) | 0.0306 (3) |
| C12 | 0.44651 (9) | 0.62379 (17) | 0.7757 (2) | 0.0339 (3) |
| C13 | 0.44373 (11) | 0.5373 (2) | 0.9203 (3) | 0.0425 (4) |
| H13 | 0.4788 | 0.5461 | 1.0165 | 0.051* |
| C14 | 0.38945 (12) | 0.4381 (2) | 0.9235 (3) | 0.0461 (5) |
| H14 | 0.3882 | 0.3786 | 1.0214 | 0.055* |
| C15 | 0.33733 (11) | 0.42539 (19) | 0.7852 (3) | 0.0437 (4) |
| H15 | 0.2998 | 0.3585 | 0.7891 | 0.052* |
| C16 | 0.34031 (10) | 0.51098 (17) | 0.6410 (3) | 0.0353 (4) |
| H16 | 0.3045 | 0.5018 | 0.5463 | 0.042* |
| C17 | 0.55036 (12) | 0.7438 (3) | 0.9090 (3) | 0.0520 (5) |
| H17A | 0.5825 | 0.6660 | 0.9222 | 0.078* |
| H17B | 0.5218 | 0.7583 | 1.0202 | 0.078* |
| H17C | 0.5825 | 0.8201 | 0.8843 | 0.078* |
| C31 | 0.34524 (9) | 0.85273 (17) | 0.0429 (2) | 0.0314 (3) |
| C32 | 0.37398 (10) | 0.96997 (18) | −0.0313 (3) | 0.0367 (4) |
| C33 | 0.34958 (11) | 1.0130 (2) | −0.1993 (3) | 0.0438 (4) |
| H33 | 0.3693 | 1.0919 | −0.2482 | 0.053* |
| C34 | 0.29652 (12) | 0.9407 (2) | −0.2952 (3) | 0.0437 (4) |
| H34 | 0.2805 | 0.9700 | −0.4102 | 0.052* |
| C35 | 0.26648 (11) | 0.82574 (19) | −0.2245 (3) | 0.0417 (4) |
| H35 | 0.2297 | 0.7772 | −0.2900 | 0.050* |
| C36 | 0.29090 (10) | 0.78266 (17) | −0.0569 (2) | 0.0354 (4) |

| | | | | |
|---|---|---|---|---|
| H36 | 0.2704 | 0.7041 | −0.0089 | 0.042* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0371 (6) | 0.0507 (8) | 0.0327 (6) | −0.0037 (5) | −0.0084 (5) | 0.0025 (6) |
| O2 | 0.0531 (8) | 0.0541 (8) | 0.0448 (8) | −0.0219 (7) | −0.0050 (7) | 0.0142 (7) |
| N1 | 0.0363 (7) | 0.0385 (7) | 0.0273 (7) | −0.0070 (6) | −0.0052 (6) | 0.0026 (6) |
| N2 | 0.0390 (7) | 0.0402 (7) | 0.0314 (8) | −0.0087 (6) | −0.0060 (6) | 0.0038 (6) |
| C1 | 0.0298 (7) | 0.0302 (7) | 0.0268 (8) | 0.0005 (6) | −0.0005 (6) | −0.0037 (6) |
| C2 | 0.0306 (7) | 0.0329 (7) | 0.0283 (8) | −0.0029 (6) | −0.0024 (6) | −0.0014 (6) |
| C3 | 0.0304 (7) | 0.0336 (8) | 0.0271 (8) | −0.0008 (6) | −0.0013 (6) | −0.0018 (6) |
| C11 | 0.0325 (7) | 0.0330 (7) | 0.0263 (7) | 0.0057 (6) | 0.0020 (6) | −0.0017 (6) |
| C12 | 0.0325 (7) | 0.0394 (8) | 0.0299 (8) | 0.0063 (6) | 0.0008 (6) | −0.0018 (7) |
| C13 | 0.0413 (9) | 0.0537 (11) | 0.0326 (9) | 0.0113 (8) | −0.0018 (7) | 0.0071 (8) |
| C14 | 0.0493 (10) | 0.0513 (11) | 0.0378 (10) | 0.0074 (8) | 0.0033 (8) | 0.0156 (9) |
| C15 | 0.0476 (9) | 0.0410 (9) | 0.0426 (11) | −0.0005 (7) | 0.0046 (8) | 0.0065 (8) |
| C16 | 0.0389 (8) | 0.0333 (8) | 0.0337 (9) | 0.0004 (7) | 0.0005 (7) | −0.0010 (7) |
| C17 | 0.0431 (10) | 0.0746 (14) | 0.0384 (11) | −0.0055 (10) | −0.0137 (8) | 0.0031 (10) |
| C31 | 0.0314 (7) | 0.0365 (8) | 0.0263 (8) | 0.0041 (6) | 0.0016 (6) | −0.0006 (6) |
| C32 | 0.0357 (8) | 0.0434 (9) | 0.0310 (9) | −0.0011 (7) | 0.0048 (7) | 0.0015 (7) |
| C33 | 0.0483 (10) | 0.0488 (10) | 0.0342 (10) | 0.0069 (8) | 0.0084 (8) | 0.0103 (8) |
| C34 | 0.0510 (10) | 0.0530 (10) | 0.0271 (8) | 0.0189 (9) | −0.0001 (7) | 0.0001 (8) |
| C35 | 0.0464 (9) | 0.0464 (9) | 0.0324 (9) | 0.0122 (7) | −0.0083 (7) | −0.0067 (8) |
| C36 | 0.0384 (8) | 0.0370 (8) | 0.0307 (8) | 0.0036 (7) | −0.0040 (7) | −0.0037 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C12 | 1.379 (2) | C14—C15 | 1.384 (3) |
| O1—C17 | 1.431 (2) | C14—H14 | 0.9500 |
| O2—C32 | 1.369 (2) | C15—C16 | 1.387 (3) |
| O2—H2 | 0.99 (4) | C15—H15 | 0.9500 |
| N1—N2 | 1.347 (2) | C16—H16 | 0.9500 |
| N1—C1 | 1.361 (2) | C17—H17A | 0.9800 |
| N1—H1 | 0.92 (3) | C17—H17B | 0.9800 |
| N2—C3 | 1.348 (2) | C17—H17C | 0.9800 |
| C1—C2 | 1.388 (2) | C31—C36 | 1.406 (2) |
| C1—C11 | 1.473 (2) | C31—C32 | 1.413 (2) |
| C2—C3 | 1.408 (2) | C32—C33 | 1.395 (3) |
| C2—H2A | 0.9500 | C33—C34 | 1.387 (3) |
| C3—C31 | 1.473 (2) | C33—H33 | 0.9500 |
| C11—C16 | 1.407 (2) | C34—C35 | 1.392 (3) |
| C11—C12 | 1.410 (2) | C34—H34 | 0.9500 |
| C12—C13 | 1.394 (3) | C35—C36 | 1.392 (3) |
| C13—C14 | 1.392 (3) | C35—H35 | 0.9500 |
| C13—H13 | 0.9500 | C36—H36 | 0.9500 |
| C12—O1—C17 | 118.24 (16) | C16—C15—H15 | 120.2 |
| C32—O2—H2 | 105 (2) | C15—C16—C11 | 121.61 (18) |

| | | | |
|---|---|---|---|
| N2—N1—C1 | 112.35 (14) | C15—C16—H16 | 119.2 |
| N2—N1—H1 | 119.2 (18) | C11—C16—H16 | 119.2 |
| C1—N1—H1 | 128.3 (18) | O1—C17—H17A | 109.5 |
| N1—N2—C3 | 105.72 (14) | O1—C17—H17B | 109.5 |
| N1—C1—C2 | 106.03 (15) | H17A—C17—H17B | 109.5 |
| N1—C1—C11 | 123.76 (15) | O1—C17—H17C | 109.5 |
| C2—C1—C11 | 130.20 (14) | H17A—C17—H17C | 109.5 |
| C1—C2—C3 | 105.82 (14) | H17B—C17—H17C | 109.5 |
| C1—C2—H2A | 127.1 | C36—C31—C32 | 117.91 (16) |
| C3—C2—H2A | 127.1 | C36—C31—C3 | 121.03 (15) |
| N2—C3—C2 | 110.08 (15) | C32—C31—C3 | 121.05 (16) |
| N2—C3—C31 | 118.85 (15) | O2—C32—C33 | 117.80 (17) |
| C2—C3—C31 | 131.07 (15) | O2—C32—C31 | 121.61 (17) |
| C16—C11—C12 | 117.79 (16) | C33—C32—C31 | 120.59 (18) |
| C16—C11—C1 | 118.49 (15) | C34—C33—C32 | 120.02 (18) |
| C12—C11—C1 | 123.71 (15) | C34—C33—H33 | 120.0 |
| O1—C12—C13 | 123.28 (17) | C32—C33—H33 | 120.0 |
| O1—C12—C11 | 116.16 (15) | C33—C34—C35 | 120.64 (18) |
| C13—C12—C11 | 120.56 (17) | C33—C34—H34 | 119.7 |
| C14—C13—C12 | 119.95 (18) | C35—C34—H34 | 119.7 |
| C14—C13—H13 | 120.0 | C36—C35—C34 | 119.34 (18) |
| C12—C13—H13 | 120.0 | C36—C35—H35 | 120.3 |
| C15—C14—C13 | 120.55 (18) | C34—C35—H35 | 120.3 |
| C15—C14—H14 | 119.7 | C35—C36—C31 | 121.49 (17) |
| C13—C14—H14 | 119.7 | C35—C36—H36 | 119.3 |
| C14—C15—C16 | 119.51 (18) | C31—C36—H36 | 119.3 |
| C14—C15—H15 | 120.2 | | |

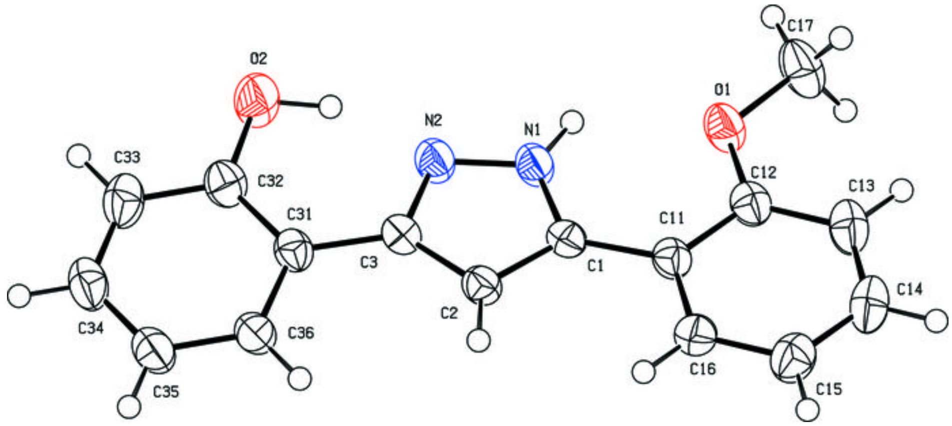
| | | | |
|---|---|---|---|
| C1—N1—N2—C3 | −0.2 (2) | C12—C13—C14—C15 | −0.9 (3) |
| N2—N1—C1—C2 | 0.46 (19) | C13—C14—C15—C16 | 1.2 (3) |
| N2—N1—C1—C11 | −178.61 (14) | C14—C15—C16—C11 | −0.1 (3) |
| N1—C1—C2—C3 | −0.50 (18) | C12—C11—C16—C15 | −1.2 (3) |
| C11—C1—C2—C3 | 178.48 (16) | C1—C11—C16—C15 | 179.75 (16) |
| N1—N2—C3—C2 | −0.1 (2) | N2—C3—C31—C36 | 172.07 (16) |
| N1—N2—C3—C31 | −179.01 (14) | C2—C3—C31—C36 | −6.5 (3) |
| C1—C2—C3—N2 | 0.4 (2) | N2—C3—C31—C32 | −7.0 (2) |
| C1—C2—C3—C31 | 179.10 (16) | C2—C3—C31—C32 | 174.43 (18) |
| N1—C1—C11—C16 | 178.05 (15) | C36—C31—C32—O2 | 178.95 (17) |
| C2—C1—C11—C16 | −0.8 (3) | C3—C31—C32—O2 | −2.0 (3) |
| N1—C1—C11—C12 | −0.9 (2) | C36—C31—C32—C33 | −0.8 (2) |
| C2—C1—C11—C12 | −179.75 (17) | C3—C31—C32—C33 | 178.21 (15) |
| C17—O1—C12—C13 | −1.8 (3) | O2—C32—C33—C34 | −179.68 (18) |
| C17—O1—C12—C11 | 178.37 (16) | C31—C32—C33—C34 | 0.1 (3) |
| C16—C11—C12—O1 | −178.60 (15) | C32—C33—C34—C35 | 0.7 (3) |
| C1—C11—C12—O1 | 0.4 (2) | C33—C34—C35—C36 | −0.8 (3) |
| C16—C11—C12—C13 | 1.5 (2) | C34—C35—C36—C31 | 0.1 (3) |
| C1—C11—C12—C13 | −179.50 (16) | C32—C31—C36—C35 | 0.8 (2) |
| O1—C12—C13—C14 | 179.62 (17) | C3—C31—C36—C35 | −178.30 (16) |
| C11—C12—C13—C14 | −0.5 (3) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···N2 | 0.99 (4) | 1.64 (4) | 2.560 (2) | 152 (3) |
| N1—H1···O1 | 0.92 (3) | 2.07 (3) | 2.628 (2) | 118 (2) |
| N1—H1···O2$^{i}$ | 0.92 (3) | 2.09 (3) | 2.892 (2) | 146 (3) |

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

**Fig. 1**


O2
N2
N1
O1
C17
C33
C32
C31
C3
C1
C11
C12
C13
C14
C34
C36
C2
C16
C35
C15