



Crystal structure of (4*Z*)-4-[(2*E*)-3-(2-chlorophenyl)-1-hydroxyprop-2-en-1-ylidene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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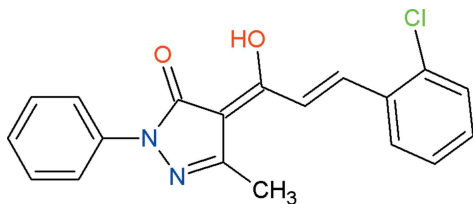
In the title compound, C₁₉H₁₅ClN₂O₂, the pyrazole ring is almost planar (r.m.s. deviation = 0.002 Å) and subtends dihedral angles of 5.31 (16) and 1.86 (16)° with the phenyl and chlorobenzene rings, respectively. An intramolecular O—H···O hydrogen bond closes an *S*(6) ring and a short C—H···O contact is also observed. In the crystal, molecules are linked by weak C—H···O interactions to generate (001) sheets. Weak aromatic π – π interactions between the chlorobenzene and pyrazole rings, with a centroid–centroid distance of 3.7956 (17) Å are also observed.

Keywords: crystal structure; pyrazole; hydrogen bonding; π – π interactions.

CCDC reference: 1400008

1. Related literature

For related structures, see: Chaudhry *et al.* (2012); Holzer *et al.* (1999); Malik *et al.* (2009).



2. Experimental

2.1. Crystal data

C ₁₉ H ₁₅ ClN ₂ O ₂	$V = 1656.41 (12) \text{ \AA}^3$
$M_r = 338.78$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 7.2348 (3) \text{ \AA}$	$\mu = 0.24 \text{ mm}^{-1}$
$b = 12.8737 (6) \text{ \AA}$	$T = 296 \text{ K}$
$c = 17.7843 (7) \text{ \AA}$	$0.34 \times 0.28 \times 0.16 \text{ mm}$

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer	8199 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	3593 independent reflections
$T_{\min} = 0.923$, $T_{\max} = 0.960$	2455 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.034$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	$\Delta\rho_{\min} = -0.17 \text{ e \AA}^{-3}$
$wR(F^2) = 0.091$	Absolute structure: Flack x
$S = 1.00$	determined using 771 quotients
3593 reflections	$[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
219 parameters	Absolute structure parameter:
H-atom parameters constrained	$-0.06 (4)$
$\Delta\rho_{\max} = 0.13 \text{ e \AA}^{-3}$	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2A···O1	0.82	1.74	2.501 (3)	154
C6—H6···O1	0.93	2.29	2.933 (4)	126
C10—H10B···O2 ⁱ	0.96	2.55	3.444 (4)	155
C16—H16···O2 ⁱⁱ	0.93	2.56	3.405 (4)	151

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

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: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7419).

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supporting information

Acta Cryst. (2015). E71, o407–o408 [doi:10.1107/S2056989015009020]

Crystal structure of (4*Z*)-4-[(2*E*)-3-(2-chlorophenyl)-1-hydroxyprop-2-en-1-ylidene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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S1. Comment

The crystal structures of 5-methyl-2-phenyl-4-((*E*)-3-phenyl-2-hydroxy-prop-2-enylidene)-1,2-dihydro-3*H*-pyrazol-3-one (Holzer *et al.*, 1999), (4*Z*)-4-((2*E*)-1-hydroxy-3-(4-methoxyphenyl)prop-2-en-1-ylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (Malik *et al.*, 2009) and (4*Z*)-4-((2*E*)-1-hydroxy-3-(3-nitrophenyl)prop-2-en-1-ylidene)-3-methyl-1-(4-methylphenyl)-1*H*-pyrazol-5(4*H*)-one (Chaudhry, *et al.*, 2012) have been published which are related to the title compound (I, Fig. 1). (I) is synthesized for the biological studies as well as for the preparation of different metal complexes.

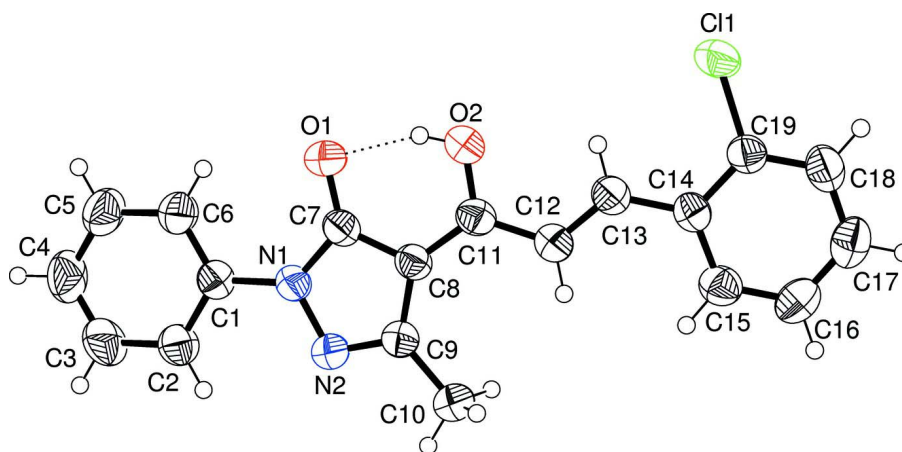
In (I), the benzene ring A (C1–C6) and the 4-[(2*E*)-3-(2-chlorophenyl)-1-hydroxyprop-2-en-1-ylidene]-5-methyl-2,4-dihydro-3*H*-pyrazol-3-one moiety (C7–C19/N1/N2/O1/O2/CL1) are planar with r. m. s. deviation of 0.0016 and 0.0158 Å, respectively. The dihedral angle between A/B is 4.87 (14)°. There exist intramolecular H-bonding of O—H···O type completing *S*(6) loop (Bernstein *et al.*, 1995). The molecules are interlinked due to C—H···O interactions (Table 1, Fig. 2). There exist π – π interactions at a distance of 3.7956 (17) Å between the centroids of Cg1—Cg2ⁱ and Cg2—Cg1ⁱⁱ [*i* = 1 + *x*, *y*, *z* and *ii* = -1 + *x*, *y*, *z*], where Cg1 and Cg2 are the centroids of heterocyclic ring C (N1/N2/C7/C8/C9) and chloro containing benzene ring D (C14–C19), respectively.

S2. Experimental

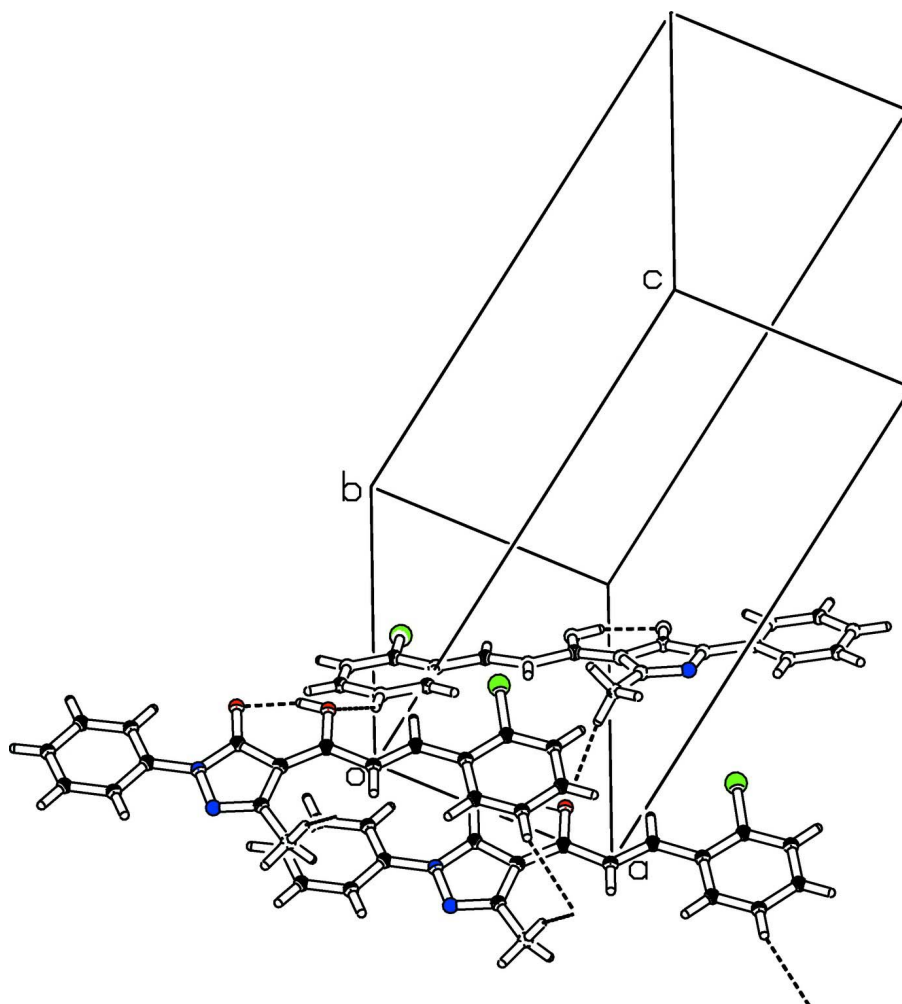
4-Acetyl-3-methyl-1-phenyl-5-hydroxypyrazole (0.218 g, 1 mmol), 2-chlorobenzaldehyde (0.211 g, 1.5 mmol) in glacial acetic acid (10 ml) and concentrated sulfuric acid (0.2 ml) was stirred at 353–360 K for 6 h. The reaction mixture was diluted with distilled water (50 ml). The precipitate was filtered, washed with methanol and dried. The crude product was purified by column chromatography using *n*-hexane and ethyl acetate mixtures as eluents. The product was recrystallized from *n*-hexane solution to afford yellow plates. Yield = 60%; m.p. 453 K

S3. Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å, O—H = 0.82 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{O})$, where $x = 1.5$ for methyl and hydroxy and $x = 1.2$ for other H-atoms.

**Figure 1**

View of the title compound with displacement ellipsoids drawn at the 50% probability level.

**Figure 2**

The partial packing, which shows that molecules are interlinked due to O—H...O bondings.

(4Z)-4-[(2E)-3-(2-Chlorophenyl)-1-hydroxyprop-2-en-1-ylidene]-3-methyl-1-phenyl-1H-pyrazol-5(4H)-one*Crystal data*C₁₉H₁₅ClN₂O₂ $M_r = 338.78$ Orthorhombic, $P2_12_12_1$ $a = 7.2348$ (3) Å $b = 12.8737$ (6) Å $c = 17.7843$ (7) Å $V = 1656.41$ (12) Å³ $Z = 4$ $F(000) = 704$ $D_x = 1.358$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2455 reflections

 $\theta = 2.3$ – 27.0° $\mu = 0.24$ mm⁻¹ $T = 296$ K

Plate, yellow

 $0.34 \times 0.28 \times 0.16$ mm*Data collection*

Bruker Kappa APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 7.70 pixels mm⁻¹ ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2005)

 $T_{\min} = 0.923$, $T_{\max} = 0.960$

8199 measured reflections

3593 independent reflections

2455 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.034$ $\theta_{\max} = 27.0^\circ$, $\theta_{\min} = 2.3^\circ$ $h = -8 \rightarrow 9$ $k = -16 \rightarrow 13$ $l = -22 \rightarrow 20$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.043$ $wR(F^2) = 0.091$ $S = 1.00$

3593 reflections

219 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0369P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.13$ e Å⁻³ $\Delta\rho_{\min} = -0.17$ e Å⁻³Absolute structure: Flack x determined using771 quotients $[(I^-)-(I^+)]/[(I^-)+(I^+)]$ (Parsons *et al.*,
2013)Absolute structure parameter: -0.06 (4)*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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.0397 (4)	0.0392 (2)	0.44274 (15)	0.0467 (7)
C2	1.1377 (5)	-0.0394 (3)	0.47830 (17)	0.0585 (9)
H2	1.0927	-0.1070	0.4786	0.070*

C3	1.3019 (5)	-0.0158 (3)	0.5130 (2)	0.0757 (11)
H3	1.3684	-0.0684	0.5366	0.091*
C4	1.3695 (5)	0.0835 (4)	0.51358 (19)	0.0788 (11)
H4	1.4806	0.0983	0.5376	0.095*
C5	1.2721 (5)	0.1611 (3)	0.47842 (19)	0.0754 (11)
H5	1.3174	0.2287	0.4786	0.091*
C6	1.1075 (5)	0.1391 (3)	0.44288 (18)	0.0612 (9)
H6	1.0421	0.1918	0.4190	0.073*
C7	0.7566 (4)	0.0745 (2)	0.36469 (16)	0.0472 (7)
C8	0.6056 (4)	0.0103 (2)	0.34325 (16)	0.0454 (7)
C9	0.6447 (4)	-0.0886 (2)	0.37664 (16)	0.0495 (7)
C10	0.5360 (5)	-0.1872 (2)	0.37362 (19)	0.0705 (10)
H10A	0.5947	-0.2387	0.4045	0.106*
H10B	0.5305	-0.2115	0.3226	0.106*
H10C	0.4130	-0.1747	0.3918	0.106*
C11	0.4645 (4)	0.0533 (2)	0.29952 (16)	0.0492 (8)
C12	0.3000 (4)	-0.0007 (3)	0.27371 (16)	0.0512 (8)
H12	0.2835	-0.0702	0.2864	0.061*
C13	0.1726 (4)	0.0468 (3)	0.23235 (17)	0.0507 (8)
H13	0.1955	0.1162	0.2212	0.061*
C14	0.0018 (4)	0.0040 (2)	0.20232 (15)	0.0455 (8)
C15	-0.0492 (5)	-0.0993 (3)	0.21263 (16)	0.0572 (8)
H15	0.0281	-0.1428	0.2400	0.069*
C16	-0.2102 (5)	-0.1386 (3)	0.18351 (18)	0.0649 (10)
H16	-0.2405	-0.2080	0.1912	0.078*
C17	-0.3274 (5)	-0.0754 (3)	0.1427 (2)	0.0672 (10)
H17	-0.4368	-0.1020	0.1232	0.081*
C18	-0.2818 (5)	0.0269 (3)	0.13120 (18)	0.0625 (9)
H18	-0.3598	0.0699	0.1036	0.075*
C19	-0.1203 (4)	0.0655 (2)	0.16072 (15)	0.0481 (8)
Cl1	-0.06694 (12)	0.19522 (6)	0.14234 (5)	0.0687 (3)
N1	0.8699 (3)	0.01404 (19)	0.40719 (13)	0.0472 (6)
N2	0.7992 (4)	-0.0870 (2)	0.41388 (14)	0.0539 (7)
O1	0.7814 (3)	0.16964 (16)	0.34743 (13)	0.0638 (6)
O2	0.4797 (3)	0.15046 (17)	0.28011 (14)	0.0659 (7)
H2A	0.5725	0.1754	0.2995	0.099*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0501 (18)	0.0511 (19)	0.0389 (15)	0.0025 (16)	-0.0027 (14)	-0.0056 (14)
C2	0.065 (2)	0.060 (2)	0.0516 (18)	0.0003 (18)	-0.0134 (17)	0.0015 (16)
C3	0.078 (3)	0.083 (3)	0.065 (2)	0.009 (2)	-0.030 (2)	0.005 (2)
C4	0.067 (2)	0.097 (3)	0.072 (2)	-0.009 (2)	-0.028 (2)	0.000 (2)
C5	0.076 (3)	0.075 (3)	0.076 (2)	-0.018 (2)	-0.020 (2)	-0.003 (2)
C6	0.063 (2)	0.059 (2)	0.062 (2)	-0.0041 (17)	-0.0131 (18)	-0.0029 (17)
C7	0.0489 (18)	0.0464 (19)	0.0461 (16)	0.0063 (15)	-0.0043 (15)	-0.0001 (15)
C8	0.0464 (18)	0.0436 (18)	0.0463 (16)	0.0051 (14)	-0.0026 (14)	-0.0017 (14)

C9	0.0484 (18)	0.0452 (18)	0.0549 (18)	0.0022 (15)	-0.0027 (15)	-0.0021 (15)
C10	0.071 (2)	0.048 (2)	0.093 (3)	-0.0056 (19)	-0.021 (2)	0.0053 (19)
C11	0.0522 (19)	0.0455 (19)	0.0500 (17)	0.0059 (16)	0.0014 (15)	-0.0019 (14)
C12	0.0507 (19)	0.049 (2)	0.0538 (17)	0.0027 (16)	-0.0040 (16)	0.0020 (16)
C13	0.049 (2)	0.051 (2)	0.0522 (17)	0.0037 (16)	-0.0020 (15)	0.0016 (15)
C14	0.0431 (18)	0.051 (2)	0.0422 (15)	0.0051 (15)	0.0016 (13)	-0.0021 (14)
C15	0.060 (2)	0.056 (2)	0.0559 (19)	0.0020 (19)	0.0010 (17)	0.0079 (16)
C16	0.067 (2)	0.060 (2)	0.068 (2)	-0.015 (2)	0.007 (2)	-0.0019 (18)
C17	0.051 (2)	0.079 (3)	0.072 (2)	-0.009 (2)	0.0011 (18)	-0.016 (2)
C18	0.053 (2)	0.070 (2)	0.064 (2)	0.0112 (18)	-0.0118 (17)	-0.0112 (19)
C19	0.0488 (18)	0.045 (2)	0.0500 (17)	0.0073 (15)	0.0004 (15)	-0.0081 (15)
C11	0.0766 (6)	0.0463 (5)	0.0832 (6)	0.0147 (5)	-0.0178 (5)	-0.0019 (5)
N1	0.0470 (15)	0.0445 (16)	0.0502 (14)	0.0025 (12)	-0.0078 (12)	-0.0009 (12)
N2	0.0547 (16)	0.0438 (16)	0.0631 (17)	-0.0022 (14)	-0.0102 (13)	0.0033 (13)
O1	0.0687 (14)	0.0432 (13)	0.0794 (15)	-0.0022 (11)	-0.0151 (13)	0.0083 (12)
O2	0.0594 (15)	0.0523 (15)	0.0860 (17)	0.0026 (11)	-0.0196 (13)	0.0104 (13)

Geometric parameters (Å, °)

C1—C6	1.377 (4)	C10—H10C	0.9600
C1—C2	1.387 (4)	C11—O2	1.302 (3)
C1—N1	1.419 (4)	C11—C12	1.453 (4)
C2—C3	1.372 (4)	C12—C13	1.328 (4)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.370 (5)	C13—C14	1.454 (4)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.373 (5)	C14—C15	1.392 (4)
C4—H4	0.9300	C14—C19	1.398 (4)
C5—C6	1.377 (4)	C15—C16	1.372 (5)
C5—H5	0.9300	C15—H15	0.9300
C6—H6	0.9300	C16—C17	1.381 (5)
C7—O1	1.276 (3)	C16—H16	0.9300
C7—N1	1.360 (3)	C17—C18	1.373 (5)
C7—C8	1.421 (4)	C17—H17	0.9300
C8—C11	1.397 (4)	C18—C19	1.374 (4)
C8—C9	1.433 (4)	C18—H18	0.9300
C9—N2	1.299 (4)	C19—C11	1.745 (3)
C9—C10	1.494 (4)	N1—N2	1.403 (3)
C10—H10A	0.9600	O2—H2A	0.8200
C10—H10B	0.9600		
C6—C1—C2	119.9 (3)	O2—C11—C8	117.8 (3)
C6—C1—N1	121.5 (3)	O2—C11—C12	116.4 (3)
C2—C1—N1	118.6 (3)	C8—C11—C12	125.8 (3)
C3—C2—C1	119.1 (3)	C13—C12—C11	121.6 (3)
C3—C2—H2	120.4	C13—C12—H12	119.2
C1—C2—H2	120.4	C11—C12—H12	119.2
C4—C3—C2	121.2 (4)	C12—C13—C14	128.2 (3)

C4—C3—H3	119.4	C12—C13—H13	115.9
C2—C3—H3	119.4	C14—C13—H13	115.9
C3—C4—C5	119.5 (4)	C15—C14—C19	116.3 (3)
C3—C4—H4	120.2	C15—C14—C13	122.6 (3)
C5—C4—H4	120.2	C19—C14—C13	121.1 (3)
C4—C5—C6	120.2 (4)	C16—C15—C14	121.9 (3)
C4—C5—H5	119.9	C16—C15—H15	119.1
C6—C5—H5	119.9	C14—C15—H15	119.1
C1—C6—C5	120.0 (3)	C15—C16—C17	120.1 (3)
C1—C6—H6	120.0	C15—C16—H16	119.9
C5—C6—H6	120.0	C17—C16—H16	119.9
O1—C7—N1	126.8 (3)	C18—C17—C16	119.8 (3)
O1—C7—C8	127.0 (3)	C18—C17—H17	120.1
N1—C7—C8	106.3 (3)	C16—C17—H17	120.1
C11—C8—C7	118.8 (3)	C17—C18—C19	119.6 (3)
C11—C8—C9	136.6 (3)	C17—C18—H18	120.2
C7—C8—C9	104.7 (3)	C19—C18—H18	120.2
N2—C9—C8	111.5 (3)	C18—C19—C14	122.4 (3)
N2—C9—C10	118.9 (3)	C18—C19—C11	117.5 (2)
C8—C9—C10	129.5 (3)	C14—C19—C11	120.1 (2)
C9—C10—H10A	109.5	C7—N1—N2	111.0 (2)
C9—C10—H10B	109.5	C7—N1—C1	129.7 (3)
H10A—C10—H10B	109.5	N2—N1—C1	119.3 (2)
C9—C10—H10C	109.5	C9—N2—N1	106.5 (2)
H10A—C10—H10C	109.5	C11—O2—H2A	109.5
H10B—C10—H10C	109.5		
C6—C1—C2—C3	-0.2 (5)	C12—C13—C14—C19	178.7 (3)
N1—C1—C2—C3	-179.9 (3)	C19—C14—C15—C16	0.1 (4)
C1—C2—C3—C4	0.5 (5)	C13—C14—C15—C16	-179.6 (3)
C2—C3—C4—C5	-0.4 (6)	C14—C15—C16—C17	-0.1 (5)
C3—C4—C5—C6	0.0 (6)	C15—C16—C17—C18	0.3 (5)
C2—C1—C6—C5	-0.1 (5)	C16—C17—C18—C19	-0.3 (5)
N1—C1—C6—C5	179.5 (3)	C17—C18—C19—C14	0.3 (5)
C4—C5—C6—C1	0.2 (5)	C17—C18—C19—C11	178.5 (2)
O1—C7—C8—C11	-1.1 (5)	C15—C14—C19—C18	-0.2 (4)
N1—C7—C8—C11	179.1 (2)	C13—C14—C19—C18	179.5 (3)
O1—C7—C8—C9	179.7 (3)	C15—C14—C19—C11	-178.3 (2)
N1—C7—C8—C9	-0.1 (3)	C13—C14—C19—C11	1.3 (4)
C11—C8—C9—N2	-179.1 (3)	O1—C7—N1—N2	-179.5 (3)
C7—C8—C9—N2	-0.1 (3)	C8—C7—N1—N2	0.3 (3)
C11—C8—C9—C10	1.1 (6)	O1—C7—N1—C1	0.2 (5)
C7—C8—C9—C10	-179.8 (3)	C8—C7—N1—C1	-180.0 (2)
C7—C8—C11—O2	0.5 (4)	C6—C1—N1—C7	5.6 (5)
C9—C8—C11—O2	179.4 (3)	C2—C1—N1—C7	-174.8 (3)
C7—C8—C11—C12	-179.1 (3)	C6—C1—N1—N2	-174.8 (3)
C9—C8—C11—C12	-0.2 (5)	C2—C1—N1—N2	4.9 (4)
O2—C11—C12—C13	0.2 (5)	C8—C9—N2—N1	0.3 (3)

C8—C11—C12—C13	179.8 (3)	C10—C9—N2—N1	-179.9 (2)
C11—C12—C13—C14	180.0 (3)	C7—N1—N2—C9	-0.4 (3)
C12—C13—C14—C15	-1.7 (5)	C1—N1—N2—C9	179.9 (2)

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O2—H2A...O1	0.82	1.74	2.501 (3)	154
C6—H6...O1	0.93	2.29	2.933 (4)	126
C10—H10B...O2 ⁱ	0.96	2.55	3.444 (4)	155
C16—H16...O2 ⁱⁱ	0.93	2.56	3.405 (4)	151

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