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Crystal structure of (4*Z*)-4-[(2*E*)-1-hydroxy-3-(naphthalen-2-yl)prop-2-en-1-ylidene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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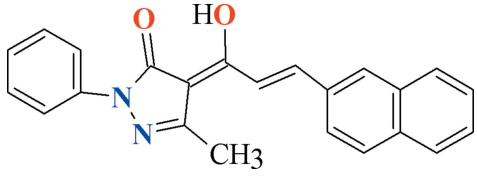
In the title compound, $C_{23}H_{18}N_2O_2$, the pyrazole ring subtends dihedral angles of 2.01 (13) and 1.55 (10)° with the pendant benzene ring and the naphthalene ring system, respectively. The molecule is almost planar (r.m.s. deviation for the 27 non-H atoms = 0.025 Å) and intramolecular O—H···O and C—H···O hydrogen bonds both close *S*(6) loops. In the crystal, very weak aromatic π–π stacking interactions between the benzene and the pyrazole rings, with centroid–centroid distances of 3.8913 (14) and 3.9285 (15) Å, are observed.

Keywords: crystal structure; pyrazole; intramolecular hydrogen bonding; π–π stacking.

CCDC reference: 1062997

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

$C_{23}H_{18}N_2O_2$ M_r = 354.39
Monoclinic, $P2_1/n$
a = 6.7067 (8) Å
b = 17.525 (2) Å
c = 15.784 (2) Å
β = 101.152 (6)°
V = 1820.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.40 × 0.16 × 0.14 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.968, T_{max} = 0.986
13979 measured reflections
3574 independent reflections
1855 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.140
S = 0.99
3574 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 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*A*···O1	0.82	1.80	2.555 (2)	153
C6—H6···O1	0.93	2.30	2.940 (3)	126

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*.

Acknowledgements

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7418).

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supporting information

Acta Cryst. (2015). E**71**, o381 [doi:10.1107/S205698901500866X]

Crystal structure of (4*Z*)-4-[(2*E*)-1-hydroxy-3-(naphthalen-2-yl)prop-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*Z*)-4-[(2*E*)-1- hydroxy-3-(naphthalen-2-yl)prop-2-en-1-ylidene]-5-methyl-2,4-dihydro-3*H* -pyrazol-3-one moiety *B* (C7 –C23/N1/N2/O1/O2) are almost planar with r.m.s. deviations of 0.0022 and 0.0179 Å, respectively. The dihedral angle between A/B is 2.30 (13)°. There exist intramolecular H-bonding of O—H···O type completing *S* (6) loop. There exist *π*–*π* interactions at a distance of 3.9285 (15) Å between the centroids of Cg1—$Cg2^{i}$ and Cg2— $Cg1^{ii}$ [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 benzene ring *A* (Fig. 2). Similarly, there exist *π*–*π* interactions at a distance of 3.8913 (14) Å between the centroids of Cg3—$Cg1^{i}$ and Cg1— $Cg3^{ii}$ [i = 1 + x, y, z and ii = -1 + x, y, z], where Cg3 is the centroids of ring *D* (C14/C15/C16/C17/C22/C23).

S2. Experimental

4-Acetyl-3-methyl-1-phenyl-5-hydroxy pyrazole (0.218 g, 1 mmol), 2-naphthaldehyde (0.234 g, 1.5 mmol) in glacial acetic acid (10 ml) and concentrated sulfuric acid (0.2 ml) was stirred at 353–360 K for 8 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 form n-hexane solution to afford purple needle. Yield = 56%, m.p. = 491 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_{iso}(H) = xU_{eq}(C, O), where x = 1.5 for methyl and hydroxy and x =1.2 for other H-atoms.

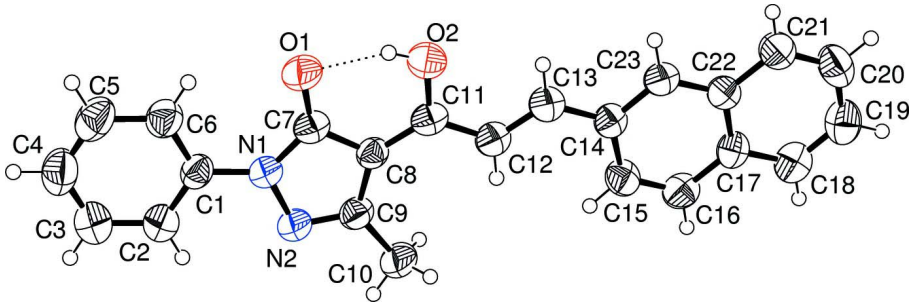

Figure 1

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

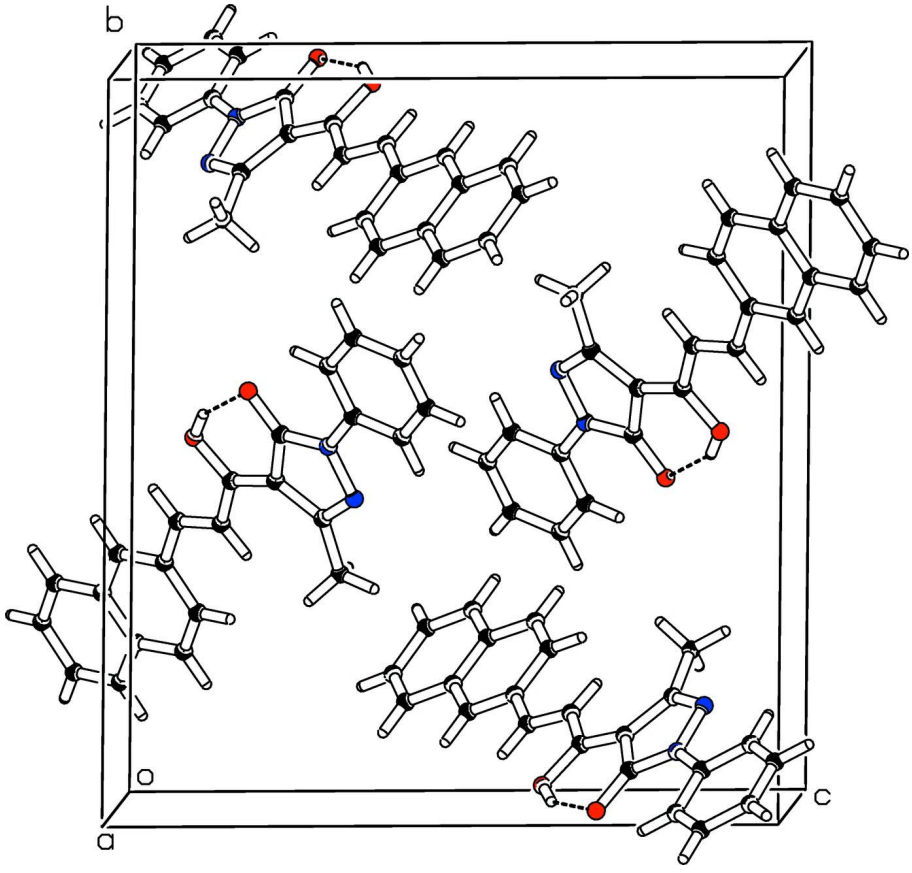

Figure 2

The partial packing, showing π–π interactions.

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Crystal data

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b = 17.525 (2) Å
c = 15.784 (2) Å
β = 101.152 (6)°
V = 1820.1 (4) Å^3
Z = 4
F(000) = 744
D_x = 1.293 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1855 reflections
θ = 2.6–26.0°

μ = 0.08 mm^{-1}
T = 296 K

Needle, purple
0.40 × 0.16 × 0.14 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.80 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.968, T_{max} = 0.986

13979 measured reflections
3574 independent reflections
1855 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 26.0°, θ_{min} = 2.6°
h = −8→5
k = −21→21
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.140
S = 0.99
3574 reflections
246 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
$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.1673 (2)	0.54343 (9)	0.17724 (11)	0.0684 (5)
O2	0.4599 (3)	0.49546 (9)	0.10912 (11)	0.0672 (5)
H2A	0.3651	0.5215	0.1186	0.101*
N1	0.1223 (3)	0.46669 (10)	0.29460 (12)	0.0527 (5)
N2	0.2155 (3)	0.40098 (11)	0.33743 (12)	0.0593 (6)
C1	−0.0446 (3)	0.49941 (13)	0.32414 (15)	0.0510 (6)
C2	−0.1094 (4)	0.46827 (15)	0.39423 (17)	0.0714 (8)
H2	−0.0430	0.4260	0.4221	0.086*
C3	−0.2734 (4)	0.49985 (18)	0.42332 (19)	0.0851 (9)
H3	−0.3152	0.4788	0.4711	0.102*
C4	−0.3740 (4)	0.56112 (17)	0.3831 (2)	0.0800 (8)
H4	−0.4843	0.5818	0.4028	0.096*
C5	−0.3108 (4)	0.59203 (15)	0.3130 (2)	0.0764 (8)

H5	−0.3794	0.6339	0.2851	0.092*
C6	−0.1459 (4)	0.56188 (14)	0.28280 (16)	0.0639 (7)
H6	−0.1040	0.5835	0.2353	0.077*
C7	0.2133 (3)	0.48753 (12)	0.22764 (15)	0.0508 (6)
C8	0.3725 (3)	0.43280 (12)	0.22720 (14)	0.0462 (6)
C9	0.3620 (3)	0.38203 (12)	0.29714 (15)	0.0533 (6)
C10	0.4899 (4)	0.31336 (14)	0.32827 (16)	0.0743 (8)
H10A	0.4788	0.2767	0.2824	0.111*
H10B	0.4434	0.2910	0.3764	0.111*
H10C	0.6293	0.3286	0.3458	0.111*
C11	0.4960 (3)	0.43911 (13)	0.16670 (15)	0.0503 (6)
C12	0.6639 (3)	0.38941 (12)	0.15888 (15)	0.0535 (6)
H12	0.6932	0.3489	0.1974	0.064*
C13	0.7796 (3)	0.39858 (13)	0.09910 (15)	0.0532 (6)
H13	0.7481	0.4397	0.0617	0.064*
C14	0.9479 (3)	0.35123 (12)	0.08677 (15)	0.0490 (6)
C15	1.0124 (4)	0.28705 (13)	0.13931 (16)	0.0590 (7)
H15	0.9461	0.2750	0.1841	0.071*
C16	1.1694 (4)	0.24273 (13)	0.12549 (17)	0.0607 (7)
H16	1.2071	0.2005	0.1606	0.073*
C17	1.2762 (3)	0.25934 (13)	0.05903 (16)	0.0519 (6)
C18	1.4400 (4)	0.21453 (14)	0.04322 (18)	0.0667 (7)
H18	1.4792	0.1716	0.0771	0.080*
C19	1.5422 (4)	0.23311 (16)	−0.02099 (19)	0.0730 (8)
H19	1.6492	0.2028	−0.0308	0.088*
C20	1.4857 (4)	0.29768 (17)	−0.07192 (18)	0.0735 (8)
H20	1.5571	0.3104	−0.1149	0.088*
C21	1.3268 (4)	0.34231 (15)	−0.05928 (16)	0.0632 (7)
H21	1.2905	0.3849	−0.0939	0.076*
C22	1.2170 (3)	0.32398 (13)	0.00630 (14)	0.0491 (6)
C23	1.0518 (3)	0.36872 (13)	0.02178 (14)	0.0518 (6)
H23	1.0121	0.4111	−0.0128	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0733 (12)	0.0593 (11)	0.0730 (12)	0.0127 (9)	0.0152 (9)	0.0219 (9)
O2	0.0714 (14)	0.0630 (12)	0.0694 (12)	0.0042 (9)	0.0190 (9)	0.0172 (10)
N1	0.0513 (13)	0.0557 (12)	0.0505 (12)	0.0075 (10)	0.0082 (10)	0.0075 (10)
N2	0.0575 (14)	0.0632 (13)	0.0577 (13)	0.0130 (11)	0.0125 (10)	0.0150 (11)
C1	0.0440 (16)	0.0540 (15)	0.0523 (15)	0.0045 (12)	0.0028 (11)	−0.0076 (12)
C2	0.066 (2)	0.0815 (19)	0.0692 (19)	0.0154 (16)	0.0189 (15)	0.0112 (16)
C3	0.079 (2)	0.103 (2)	0.079 (2)	0.0145 (19)	0.0293 (17)	0.0075 (18)
C4	0.067 (2)	0.086 (2)	0.089 (2)	0.0127 (18)	0.0177 (17)	−0.0186 (19)
C5	0.073 (2)	0.0635 (18)	0.088 (2)	0.0187 (15)	0.0044 (16)	−0.0115 (17)
C6	0.0651 (18)	0.0612 (16)	0.0645 (17)	0.0099 (14)	0.0105 (13)	−0.0034 (14)
C7	0.0488 (16)	0.0475 (14)	0.0535 (15)	−0.0038 (12)	0.0029 (12)	0.0040 (12)
C8	0.0389 (14)	0.0490 (14)	0.0491 (14)	−0.0021 (12)	0.0051 (11)	0.0045 (11)

C9	0.0494 (16)	0.0521 (14)	0.0568 (15)	0.0034 (12)	0.0065 (12)	0.0079 (13)
C10	0.0706 (19)	0.0756 (18)	0.0787 (19)	0.0235 (15)	0.0194 (14)	0.0298 (15)
C11	0.0480 (16)	0.0451 (14)	0.0533 (15)	−0.0085 (12)	−0.0013 (12)	0.0003 (12)
C12	0.0501 (16)	0.0504 (14)	0.0584 (16)	−0.0051 (13)	0.0064 (12)	0.0034 (12)
C13	0.0521 (16)	0.0483 (14)	0.0581 (16)	−0.0096 (12)	0.0081 (12)	0.0002 (12)
C14	0.0445 (15)	0.0464 (14)	0.0552 (15)	−0.0089 (12)	0.0076 (12)	−0.0017 (12)
C15	0.0578 (17)	0.0536 (15)	0.0682 (17)	−0.0082 (13)	0.0185 (13)	0.0080 (13)
C16	0.0576 (17)	0.0504 (15)	0.0726 (18)	−0.0062 (14)	0.0088 (13)	0.0127 (13)
C17	0.0431 (15)	0.0480 (14)	0.0632 (17)	−0.0093 (12)	0.0070 (12)	−0.0082 (12)
C18	0.0623 (19)	0.0541 (16)	0.082 (2)	−0.0060 (14)	0.0104 (15)	−0.0042 (14)
C19	0.0643 (19)	0.0697 (19)	0.087 (2)	−0.0030 (15)	0.0187 (16)	−0.0200 (17)
C20	0.070 (2)	0.089 (2)	0.0660 (19)	−0.0130 (17)	0.0261 (15)	−0.0147 (17)
C21	0.0609 (18)	0.0693 (17)	0.0593 (17)	−0.0065 (15)	0.0113 (13)	−0.0028 (14)
C22	0.0466 (16)	0.0519 (15)	0.0475 (14)	−0.0113 (13)	0.0057 (11)	−0.0056 (12)
C23	0.0496 (16)	0.0482 (14)	0.0554 (16)	−0.0064 (12)	0.0042 (12)	0.0039 (12)

Geometric parameters (Å, º)

O1—C7	1.262 (2)	C10—H10C	0.9600
O2—C11	1.332 (2)	C11—C12	1.447 (3)
O2—H2A	0.8200	C12—C13	1.342 (3)
N1—C7	1.368 (3)	C12—H12	0.9300
N1—C1	1.415 (3)	C13—C14	1.444 (3)
N1—N2	1.418 (2)	C13—H13	0.9300
N2—C9	1.312 (3)	C14—C23	1.381 (3)
C1—C2	1.377 (3)	C14—C15	1.414 (3)
C1—C6	1.383 (3)	C15—C16	1.360 (3)
C2—C3	1.387 (3)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.410 (3)
C3—C4	1.359 (4)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.412 (3)
C4—C5	1.371 (4)	C17—C22	1.416 (3)
C4—H4	0.9300	C18—C19	1.368 (3)
C5—C6	1.390 (3)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.397 (3)
C6—H6	0.9300	C19—H19	0.9300
C7—C8	1.436 (3)	C20—C21	1.368 (3)
C8—C11	1.385 (3)	C20—H20	0.9300
C8—C9	1.430 (3)	C21—C22	1.418 (3)
C9—C10	1.504 (3)	C21—H21	0.9300
C10—H10A	0.9600	C22—C23	1.417 (3)
C10—H10B	0.9600	C23—H23	0.9300
C11—O2—H2A	109.5	O2—C11—C12	115.5 (2)
C7—N1—C1	130.2 (2)	C8—C11—C12	126.1 (2)
C7—N1—N2	111.32 (18)	C13—C12—C11	123.6 (2)
C1—N1—N2	118.43 (19)	C13—C12—H12	118.2
C9—N2—N1	106.08 (18)	C11—C12—H12	118.2

C2—C1—C6	119.4 (2)	C12—C13—C14	126.8 (2)
C2—C1—N1	119.8 (2)	C12—C13—H13	116.6
C6—C1—N1	120.8 (2)	C14—C13—H13	116.6
C1—C2—C3	120.1 (3)	C23—C14—C15	118.1 (2)
C1—C2—H2	119.9	C23—C14—C13	119.5 (2)
C3—C2—H2	119.9	C15—C14—C13	122.4 (2)
C4—C3—C2	121.0 (3)	C16—C15—C14	121.2 (2)
C4—C3—H3	119.5	C16—C15—H15	119.4
C2—C3—H3	119.5	C14—C15—H15	119.4
C3—C4—C5	119.1 (3)	C15—C16—C17	121.5 (2)
C3—C4—H4	120.4	C15—C16—H16	119.3
C5—C4—H4	120.4	C17—C16—H16	119.3
C4—C5—C6	121.1 (3)	C16—C17—C18	122.8 (2)
C4—C5—H5	119.4	C16—C17—C22	118.5 (2)
C6—C5—H5	119.4	C18—C17—C22	118.7 (2)
C1—C6—C5	119.3 (3)	C19—C18—C17	121.1 (3)
C1—C6—H6	120.3	C19—C18—H18	119.4
C5—C6—H6	120.3	C17—C18—H18	119.4
O1—C7—N1	127.1 (2)	C18—C19—C20	120.0 (3)
O1—C7—C8	127.3 (2)	C18—C19—H19	120.0
N1—C7—C8	105.57 (19)	C20—C19—H19	120.0
C11—C8—C9	135.0 (2)	C21—C20—C19	120.8 (3)
C11—C8—C7	119.6 (2)	C21—C20—H20	119.6
C9—C8—C7	105.3 (2)	C19—C20—H20	119.6
N2—C9—C8	111.71 (19)	C20—C21—C22	120.4 (2)
N2—C9—C10	118.5 (2)	C20—C21—H21	119.8
C8—C9—C10	129.8 (2)	C22—C21—H21	119.8
C9—C10—H10A	109.5	C17—C22—C23	118.8 (2)
C9—C10—H10B	109.5	C17—C22—C21	118.9 (2)
H10A—C10—H10B	109.5	C23—C22—C21	122.3 (2)
C9—C10—H10C	109.5	C14—C23—C22	121.9 (2)
H10A—C10—H10C	109.5	C14—C23—H23	119.0
H10B—C10—H10C	109.5	C22—C23—H23	119.0
O2—C11—C8	118.4 (2)		

C7—N1—N2—C9	0.1 (2)	C7—C8—C11—O2	−1.4 (3)
C1—N1—N2—C9	179.18 (19)	C9—C8—C11—C12	0.3 (4)
C7—N1—C1—C2	−179.6 (2)	C7—C8—C11—C12	178.99 (19)
N2—N1—C1—C2	1.5 (3)	O2—C11—C12—C13	0.8 (3)
C7—N1—C1—C6	1.2 (4)	C8—C11—C12—C13	−179.6 (2)
N2—N1—C1—C6	−177.66 (19)	C11—C12—C13—C14	−179.44 (19)
C6—C1—C2—C3	−0.6 (4)	C12—C13—C14—C23	−180.0 (2)
N1—C1—C2—C3	−179.7 (2)	C12—C13—C14—C15	−0.2 (4)
C1—C2—C3—C4	0.7 (4)	C23—C14—C15—C16	−1.3 (3)
C2—C3—C4—C5	−0.3 (4)	C13—C14—C15—C16	179.0 (2)
C3—C4—C5—C6	−0.2 (4)	C14—C15—C16—C17	0.8 (4)
C2—C1—C6—C5	0.1 (3)	C15—C16—C17—C18	179.8 (2)
N1—C1—C6—C5	179.3 (2)	C15—C16—C17—C22	0.2 (3)

C4—C5—C6—C1	0.3 (4)	C16—C17—C18—C19	−178.9 (2)
C1—N1—C7—O1	1.4 (4)	C22—C17—C18—C19	0.7 (3)
N2—N1—C7—O1	−179.63 (19)	C17—C18—C19—C20	0.4 (4)
C1—N1—C7—C8	−178.9 (2)	C18—C19—C20—C21	−1.0 (4)
N2—N1—C7—C8	0.0 (2)	C19—C20—C21—C22	0.4 (4)
O1—C7—C8—C11	0.5 (3)	C16—C17—C22—C23	−0.7 (3)
N1—C7—C8—C11	−179.13 (19)	C18—C17—C22—C23	179.63 (19)
O1—C7—C8—C9	179.5 (2)	C16—C17—C22—C21	178.4 (2)
N1—C7—C8—C9	−0.1 (2)	C18—C17—C22—C21	−1.3 (3)
N1—N2—C9—C8	−0.2 (2)	C20—C21—C22—C17	0.7 (3)
N1—N2—C9—C10	−179.94 (18)	C20—C21—C22—C23	179.8 (2)
C11—C8—C9—N2	179.0 (2)	C15—C14—C23—C22	0.7 (3)
C7—C8—C9—N2	0.2 (3)	C13—C14—C23—C22	−179.51 (18)
C11—C8—C9—C10	−1.3 (4)	C17—C22—C23—C14	0.2 (3)
C7—C8—C9—C10	179.9 (2)	C21—C22—C23—C14	−178.8 (2)
C9—C8—C11—O2	179.9 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O1	0.82	1.80	2.555 (2)	153
C6—H6···O1	0.93	2.30	2.940 (3)	126