



IUCrData

ISSN 2414-3146

(E)-1-(3,4-Dimethoxyphenyl)-3-(1,3-diphenyl-1H-pyrazol-4-yl)prop-2-en-1-one

Jiha Sung*

Department of Applied Chemistry, Dongduk Women's University, Seoul 136-714, Republic of Korea. *Correspondence e-mail: dddklab@gmail.com

Received 28 August 2024

Accepted 3 September 2024

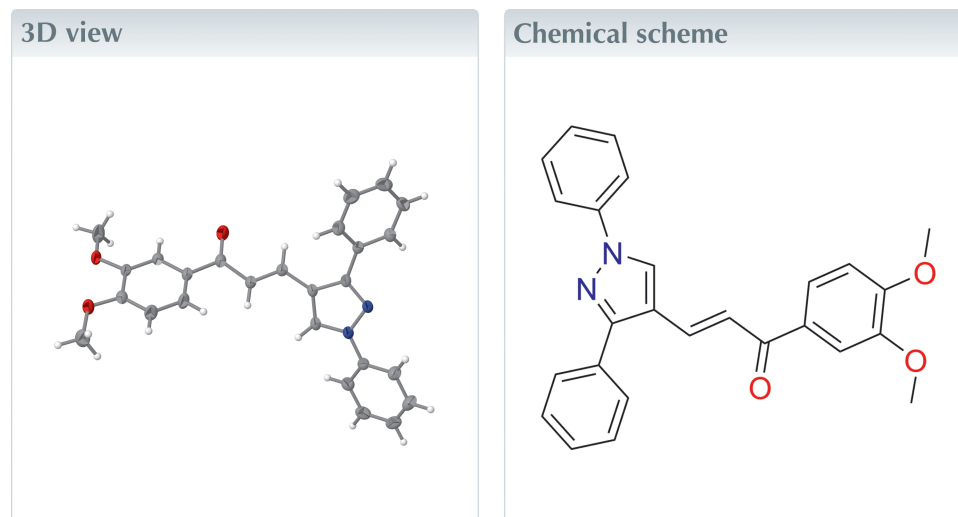
Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

Keywords: crystal structure; pyrazole; chalcone; C—H···O hydrogen bonds.

CCDC reference: 2381555

Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{26}H_{22}N_2O_3$, the dihedral angle between the benzene and pyrazole rings of the chalcone unit is $88.3(1)^\circ$. The pyrazole ring has two attached phenyl rings that form dihedral angles with the pyrazole ring of $22.6(2)$ and $40.0(1)^\circ$. In the crystal, pairwise C—H···O hydrogen bonds generate $R_2^2(20)$ inversion dimers.



Structure description

Pyrazoles are promising scaffolds in medicinal chemistry due to their versatile biological efficacy, including antibacterial, anti-inflammatory, antioxidant, antidepressant, and anticancer activity (Brullo *et al.*, 2020; Ebenezer *et al.*, 2022). As a result of intensive research on the anticancer activity of pyrazole-containing molecules, a number of anticancer drugs such as niraparib, crinitib and darolutamide have been developed and are commercially available (Sivaramakarthikeyan *et al.*, 2020). Chalcones also exhibit various physiological phenomena, including anticancer activity (Elkanzi *et al.*, 2022). As part of our ongoing research to develop new chalcones derivatives (Sung, 2019) with anti-cancer activities, the pyrazole-containing chalcone title compound was synthesized and its crystal structure was determined.

The title compound, $C_{26}H_{22}N_2O_3$, was prepared by a Claisen–Schmidt condensation reaction between 3,4-dimethoxyacetophenone and 1,3-diphenyl-1H-pyrazole-4-carbaldehyde (Fig. 1). The molecular structure of title compound is shown in Fig. 2. The C=C and C=O double bonds usually lie in the same plane in the enone bridge of the chalcone unit. However, in this molecule, the O1—C1—C8—C9 torsion angle is $17.3(2)^\circ$, indicating a significant twist. The C2—C7 benzene ring has two methoxy groups attached at C4 and C5, which are twisted from the ring plane with torsion angles of $6.1(2)^\circ$ [C3—C4—O2—C10] and $-7.3(2)^\circ$ [C6—C5—O3—C11]. The pyrazole ring (N1/N2/C14/C12/C13) has the C15—C20 and C21—C26 phenyl groups attached to atoms N1 and C14, respectively. The C15—C20 and C21—C26 phenyl rings make dihedral angles with the pyrazole ring of

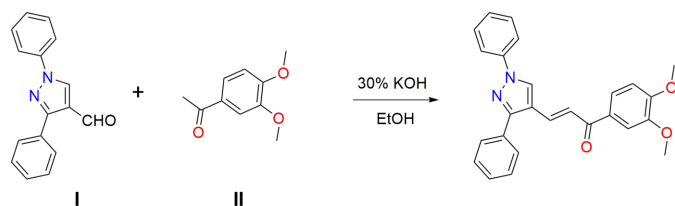


Figure 1
Synthetic scheme for the title compound.

22.6 (2) and 40.0 (1)°, respectively, while the dihedral angle between the phenyl rings is 53.3 (3)°. In the crystal, pairs of C—H···O hydrogen bonds generate inversion dimers with graph-set notation $R_2^2(20)$ (Table 1, Fig. 3).

Synthesis and crystallization

3,4-Dimethoxyacetophenone (180 mg, 1 mmol) was dissolved in 20 ml of ethanol. Then, 1,3-diphenyl-1*H*-pyrazole-4-carbaldehyde (248 mg, 1 mmol) was slowly added until a clear solution was formed. The temperature of reaction mixture was adjusted to 276–277 K using an ice bath. To the cooled reaction mixture was added 1.5 ml of 30% aqueous KOH solution, and the reaction mixture was stirred at room temperature for 30 h. This mixture was poured into iced water (50 ml) and was acidified (pH = 3) with 3 *N* HCl solution to give a precipitate. After filtration, the crude solid was recrystallized from ethanol solution to form crystals in the form of yellow blocks suitable for X-ray diffraction.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

This work was supported by a Dongduk Women's University grant.

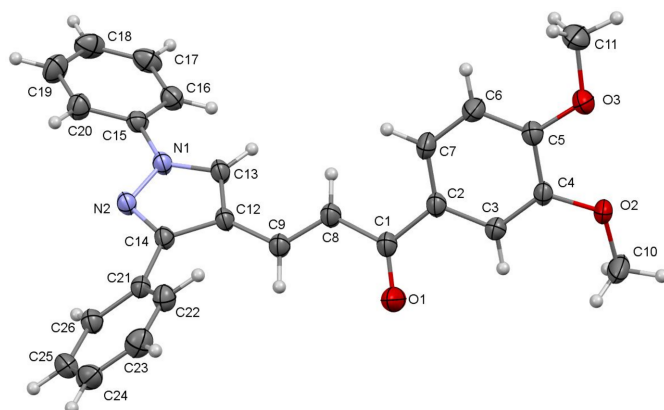


Figure 2
The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

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

<i>D</i> — <i>H</i> ··· <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> — <i>H</i> ··· <i>A</i>
C13—H13···O2 ⁱ	0.94	2.34	3.2648 (19)	169

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

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₆ H ₂₂ N ₂ O ₃
<i>M_r</i>	410.45
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	223
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.342 (3), 10.524 (3), 11.967 (4)
α , β , γ (°)	73.831 (10), 79.643 (11), 72.648 (10)
<i>V</i> (Å ³)	1072.6 (6)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.26 × 0.22 × 0.07
Data collection	
Diffractometer	PHOTON III M14
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.706, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	39655, 5269, 4173
<i>R_{int}</i>	0.044
(sin θ/ <i>λ</i>) _{max} (Å ⁻¹)	0.667
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.044, 0.115, 1.04
No. of reflections	5269
No. of parameters	282
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.24, -0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

References

- Bruker (2012). *APEX2* and *SAINT*. Bruker AXS Inc. Madison, Wisconsin, USA.
- Brullo, C., Rapetti, F. & Bruno, O. (2020). *Molecules*, **25**, 3457.
- Ebenezer, O., Shapi, M. & Tuszyński, J. (2022). *Biomedicines*, **10**, 1124.

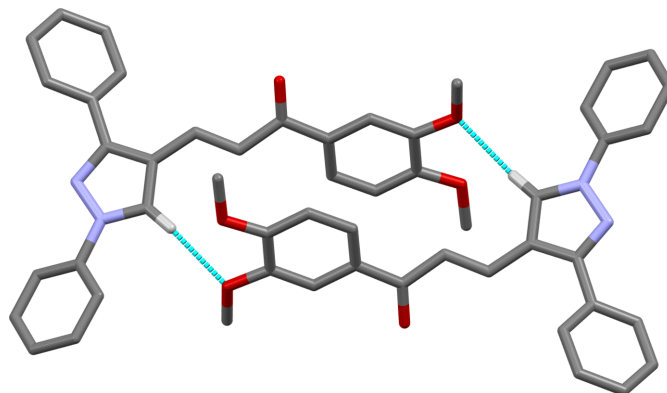


Figure 3
Part of the crystal structure of the title compound, showing the weak C—H···O pairwise hydrogen bonds that form $R_2^2(20)$ dimers.

- Elkanzi, N. A. A., Hrichi, H., Alolayan, R. A., Derafa, W., Zahou, F. M. & Bakr, R. B. (2022). *ACS Omega*, **7**, 27769–27786.
- Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Sivaramakarthykeyan, R., Iniyaval, S., Saravanan, V., Lim, W.-M., Mai, C.-W. & Ramalingan, C. (2020). *ACS Omega*, **5**, 10089–10098.
- Sung, J. (2019). *IUCrData*, **4**, x191281.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2024). **9**, x240866 [https://doi.org/10.1107/S2414314624008666]

(*E*)-1-(3,4-Dimethoxyphenyl)-3-(1,3-diphenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one

Jiha Sung

(*E*)-1-(3,4-Dimethoxyphenyl)-3-(1,3-diphenyl-1*H*-pyrazol-4-yl)prop-2-en-1-one*Crystal data*

$C_{26}H_{22}N_2O_3$	$Z = 2$
$M_r = 410.45$	$F(000) = 432$
Triclinic, $P\bar{1}$	$D_x = 1.271 \text{ Mg m}^{-3}$
$a = 9.342 (3) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 10.524 (3) \text{ \AA}$	Cell parameters from 9940 reflections
$c = 11.967 (4) \text{ \AA}$	$\theta = 2.3\text{--}28.2^\circ$
$\alpha = 73.831 (10)^\circ$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 79.643 (11)^\circ$	$T = 223 \text{ K}$
$\gamma = 72.648 (10)^\circ$	BLOCK, yellow
$V = 1072.6 (6) \text{ \AA}^3$	$0.26 \times 0.22 \times 0.07 \text{ mm}$

Data collection

PHOTON III M14 diffractometer	5269 independent reflections
φ and ω scans	4173 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Krause <i>et al.</i> , 2015)	$R_{\text{int}} = 0.044$
$T_{\text{min}} = 0.706$, $T_{\text{max}} = 0.746$	$\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 2.1^\circ$
39655 measured reflections	$h = -12 \rightarrow 12$
	$k = -13 \rightarrow 13$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.3885P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
5269 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
282 parameters	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.62809 (17)	0.71283 (14)	0.49957 (12)	0.0323 (3)
C2	0.67643 (16)	0.84296 (13)	0.47121 (12)	0.0289 (3)
C3	0.70448 (15)	0.90841 (13)	0.35225 (11)	0.0278 (3)
H3	0.6908	0.8711	0.2934	0.033*
C4	0.75205 (14)	1.02730 (13)	0.32222 (11)	0.0256 (3)
C5	0.77516 (16)	1.08293 (13)	0.41023 (12)	0.0289 (3)
C6	0.74834 (19)	1.01806 (16)	0.52704 (13)	0.0380 (3)
H6	0.7640	1.0540	0.5861	0.046*
C7	0.69805 (18)	0.89929 (15)	0.55667 (12)	0.0367 (3)
H7	0.6785	0.8568	0.6360	0.044*
C8	0.55681 (16)	0.66700 (14)	0.61955 (12)	0.0305 (3)
H8	0.5185	0.7306	0.6663	0.037*
C9	0.54487 (16)	0.53814 (14)	0.66390 (12)	0.0299 (3)
H9	0.5866	0.4748	0.6172	0.036*
C10	0.7475 (2)	1.05899 (18)	0.11652 (13)	0.0506 (5)
H10A	0.8065	0.9658	0.1172	0.076*
H10B	0.7719	1.1196	0.0427	0.076*
H10C	0.6410	1.0632	0.1260	0.076*
C11	0.8254 (2)	1.27120 (18)	0.45672 (15)	0.0502 (4)
H11A	0.7316	1.2800	0.5078	0.075*
H11B	0.8386	1.3616	0.4178	0.075*
H11C	0.9089	1.2194	0.5026	0.075*
C12	0.47133 (15)	0.49005 (13)	0.77989 (12)	0.0276 (3)
C13	0.35511 (16)	0.56706 (13)	0.84202 (12)	0.0301 (3)
H13	0.3103	0.6616	0.8181	0.036*
C14	0.49721 (15)	0.35452 (13)	0.85328 (11)	0.0254 (3)
C15	0.19811 (15)	0.51457 (13)	1.03298 (12)	0.0274 (3)
C16	0.07757 (16)	0.62931 (14)	1.00652 (13)	0.0336 (3)
H16	0.0756	0.6874	0.9309	0.040*
C17	-0.04030 (17)	0.65744 (16)	1.09308 (15)	0.0397 (4)
H17	-0.1219	0.7351	1.0755	0.048*
C18	-0.03903 (19)	0.57258 (17)	1.20473 (15)	0.0439 (4)
H18	-0.1196	0.5915	1.2625	0.053*
C19	0.08327 (19)	0.45892 (18)	1.23016 (14)	0.0440 (4)
H19	0.0855	0.4014	1.3060	0.053*
C20	0.20220 (17)	0.42922 (15)	1.14506 (13)	0.0356 (3)
H20	0.2845	0.3523	1.1631	0.043*
C21	0.61238 (15)	0.22895 (13)	0.83440 (11)	0.0257 (3)
C22	0.75946 (16)	0.23372 (14)	0.78641 (12)	0.0324 (3)
H22	0.7839	0.3184	0.7613	0.039*
C23	0.86940 (17)	0.11392 (16)	0.77567 (14)	0.0389 (3)
H23	0.9679	0.1181	0.7436	0.047*
C24	0.83513 (18)	-0.01186 (15)	0.81191 (13)	0.0395 (4)
H24	0.9101	-0.0925	0.8046	0.047*
C25	0.68948 (18)	-0.01789 (14)	0.85903 (13)	0.0371 (3)

H25	0.6657	-0.1028	0.8837	0.045*
C26	0.57853 (16)	0.10188 (13)	0.86983 (12)	0.0310 (3)
H26	0.4800	0.0972	0.9012	0.037*
N1	0.31718 (13)	0.48180 (11)	0.94375 (10)	0.0276 (2)
N2	0.40423 (12)	0.34957 (11)	0.95287 (10)	0.0271 (2)
O1	0.64801 (16)	0.64685 (12)	0.42551 (10)	0.0540 (3)
O2	0.78144 (12)	1.10062 (9)	0.21009 (8)	0.0311 (2)
O3	0.82098 (12)	1.20091 (10)	0.37080 (9)	0.0362 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0405 (8)	0.0263 (7)	0.0269 (7)	-0.0117 (6)	0.0029 (6)	-0.0019 (5)
C2	0.0330 (7)	0.0244 (6)	0.0253 (6)	-0.0089 (5)	0.0017 (5)	-0.0012 (5)
C3	0.0329 (7)	0.0256 (6)	0.0234 (6)	-0.0089 (5)	0.0005 (5)	-0.0047 (5)
C4	0.0267 (6)	0.0222 (6)	0.0222 (6)	-0.0045 (5)	0.0012 (5)	-0.0006 (5)
C5	0.0325 (7)	0.0257 (6)	0.0277 (7)	-0.0102 (5)	-0.0007 (5)	-0.0037 (5)
C6	0.0557 (10)	0.0390 (8)	0.0243 (7)	-0.0222 (7)	-0.0021 (6)	-0.0063 (6)
C7	0.0525 (9)	0.0354 (8)	0.0216 (6)	-0.0198 (7)	0.0000 (6)	0.0008 (6)
C8	0.0355 (7)	0.0252 (6)	0.0269 (7)	-0.0091 (5)	0.0039 (6)	-0.0033 (5)
C9	0.0336 (7)	0.0251 (6)	0.0269 (7)	-0.0071 (5)	0.0020 (5)	-0.0035 (5)
C10	0.0866 (14)	0.0502 (10)	0.0237 (7)	-0.0381 (10)	-0.0088 (8)	0.0007 (7)
C11	0.0754 (13)	0.0474 (10)	0.0415 (9)	-0.0368 (9)	0.0012 (8)	-0.0146 (8)
C12	0.0328 (7)	0.0203 (6)	0.0266 (6)	-0.0085 (5)	0.0000 (5)	-0.0014 (5)
C13	0.0361 (7)	0.0208 (6)	0.0289 (7)	-0.0081 (5)	0.0008 (6)	-0.0009 (5)
C14	0.0275 (6)	0.0222 (6)	0.0253 (6)	-0.0090 (5)	-0.0008 (5)	-0.0020 (5)
C15	0.0290 (7)	0.0255 (6)	0.0285 (7)	-0.0102 (5)	0.0020 (5)	-0.0076 (5)
C16	0.0343 (8)	0.0278 (7)	0.0371 (8)	-0.0071 (6)	-0.0020 (6)	-0.0073 (6)
C17	0.0315 (8)	0.0339 (8)	0.0538 (10)	-0.0054 (6)	0.0012 (7)	-0.0180 (7)
C18	0.0381 (8)	0.0480 (9)	0.0481 (9)	-0.0162 (7)	0.0150 (7)	-0.0226 (8)
C19	0.0468 (9)	0.0492 (9)	0.0315 (8)	-0.0161 (8)	0.0083 (7)	-0.0064 (7)
C20	0.0360 (8)	0.0334 (7)	0.0314 (7)	-0.0068 (6)	0.0016 (6)	-0.0040 (6)
C21	0.0298 (7)	0.0237 (6)	0.0208 (6)	-0.0063 (5)	-0.0023 (5)	-0.0020 (5)
C22	0.0322 (7)	0.0310 (7)	0.0313 (7)	-0.0098 (6)	-0.0012 (6)	-0.0030 (6)
C23	0.0297 (7)	0.0439 (9)	0.0357 (8)	-0.0026 (6)	-0.0002 (6)	-0.0075 (7)
C24	0.0425 (9)	0.0327 (8)	0.0347 (8)	0.0061 (6)	-0.0071 (7)	-0.0096 (6)
C25	0.0512 (9)	0.0237 (7)	0.0338 (8)	-0.0071 (6)	-0.0055 (7)	-0.0050 (6)
C26	0.0344 (7)	0.0268 (7)	0.0304 (7)	-0.0100 (6)	-0.0013 (6)	-0.0039 (5)
N1	0.0308 (6)	0.0202 (5)	0.0271 (6)	-0.0055 (4)	0.0004 (5)	-0.0019 (4)
N2	0.0288 (6)	0.0197 (5)	0.0279 (6)	-0.0051 (4)	0.0008 (4)	-0.0020 (4)
O1	0.0929 (10)	0.0427 (6)	0.0342 (6)	-0.0384 (7)	0.0159 (6)	-0.0134 (5)
O2	0.0460 (6)	0.0264 (5)	0.0203 (4)	-0.0153 (4)	-0.0013 (4)	0.0004 (4)
O3	0.0517 (6)	0.0316 (5)	0.0299 (5)	-0.0223 (5)	0.0001 (5)	-0.0050 (4)

Geometric parameters (Å, °)

C1—O1	1.2283 (18)	C13—N1	1.3560 (17)
C1—C8	1.4832 (19)	C13—H13	0.9400

C1—C2	1.4998 (19)	C14—N2	1.3408 (17)
C2—C7	1.386 (2)	C14—C21	1.4784 (18)
C2—C3	1.4133 (18)	C15—C16	1.390 (2)
C3—C4	1.3842 (18)	C15—C20	1.391 (2)
C3—H3	0.9400	C15—N1	1.4302 (17)
C4—O2	1.3743 (15)	C16—C17	1.393 (2)
C4—C5	1.4139 (19)	C16—H16	0.9400
C5—O3	1.3659 (16)	C17—C18	1.385 (2)
C5—C6	1.3884 (19)	C17—H17	0.9400
C6—C7	1.397 (2)	C18—C19	1.391 (2)
C6—H6	0.9400	C18—H18	0.9400
C7—H7	0.9400	C19—C20	1.390 (2)
C8—C9	1.3422 (18)	C19—H19	0.9400
C8—H8	0.9400	C20—H20	0.9400
C9—C12	1.4588 (19)	C21—C26	1.3988 (18)
C9—H9	0.9400	C21—C22	1.4005 (19)
C10—O2	1.4249 (19)	C22—C23	1.390 (2)
C10—H10A	0.9700	C22—H22	0.9400
C10—H10B	0.9700	C23—C24	1.388 (2)
C10—H10C	0.9700	C23—H23	0.9400
C11—O3	1.4363 (19)	C24—C25	1.389 (2)
C11—H11A	0.9700	C24—H24	0.9400
C11—H11B	0.9700	C25—C26	1.394 (2)
C11—H11C	0.9700	C25—H25	0.9400
C12—C13	1.3817 (19)	C26—H26	0.9400
C12—C14	1.4274 (17)	N1—N2	1.3719 (15)
O1—C1—C8	121.61 (13)	N2—C14—C12	111.62 (11)
O1—C1—C2	120.66 (12)	N2—C14—C21	119.59 (11)
C8—C1—C2	117.73 (12)	C12—C14—C21	128.73 (12)
C7—C2—C3	118.98 (12)	C16—C15—C20	120.49 (13)
C7—C2—C1	122.70 (12)	C16—C15—N1	119.88 (12)
C3—C2—C1	118.31 (12)	C20—C15—N1	119.61 (12)
C4—C3—C2	120.18 (12)	C15—C16—C17	119.35 (14)
C4—C3—H3	119.9	C15—C16—H16	120.3
C2—C3—H3	119.9	C17—C16—H16	120.3
O2—C4—C3	125.50 (12)	C18—C17—C16	120.93 (14)
O2—C4—C5	114.22 (11)	C18—C17—H17	119.5
C3—C4—C5	120.28 (12)	C16—C17—H17	119.5
O3—C5—C6	125.18 (13)	C17—C18—C19	119.00 (14)
O3—C5—C4	115.36 (11)	C17—C18—H18	120.5
C6—C5—C4	119.45 (12)	C19—C18—H18	120.5
C5—C6—C7	119.92 (14)	C20—C19—C18	120.95 (15)
C5—C6—H6	120.0	C20—C19—H19	119.5
C7—C6—H6	120.0	C18—C19—H19	119.5
C2—C7—C6	121.18 (13)	C19—C20—C15	119.26 (14)
C2—C7—H7	119.4	C19—C20—H20	120.4
C6—C7—H7	119.4	C15—C20—H20	120.4

C9—C8—C1	122.51 (13)	C26—C21—C22	118.70 (12)
C9—C8—H8	118.7	C26—C21—C14	120.51 (12)
C1—C8—H8	118.7	C22—C21—C14	120.71 (12)
C8—C9—C12	124.25 (13)	C23—C22—C21	120.31 (13)
C8—C9—H9	117.9	C23—C22—H22	119.8
C12—C9—H9	117.9	C21—C22—H22	119.8
O2—C10—H10A	109.5	C24—C23—C22	120.61 (14)
O2—C10—H10B	109.5	C24—C23—H23	119.7
H10A—C10—H10B	109.5	C22—C23—H23	119.7
O2—C10—H10C	109.5	C23—C24—C25	119.64 (13)
H10A—C10—H10C	109.5	C23—C24—H24	120.2
H10B—C10—H10C	109.5	C25—C24—H24	120.2
O3—C11—H11A	109.5	C24—C25—C26	120.07 (14)
O3—C11—H11B	109.5	C24—C25—H25	120.0
H11A—C11—H11B	109.5	C26—C25—H25	120.0
O3—C11—H11C	109.5	C25—C26—C21	120.66 (14)
H11A—C11—H11C	109.5	C25—C26—H26	119.7
H11B—C11—H11C	109.5	C21—C26—H26	119.7
C13—C12—C14	104.13 (11)	C13—N1—N2	111.93 (11)
C13—C12—C9	126.94 (12)	C13—N1—C15	127.64 (11)
C14—C12—C9	128.89 (12)	N2—N1—C15	120.36 (10)
N1—C13—C12	107.76 (12)	C14—N2—N1	104.55 (10)
N1—C13—H13	126.1	C4—O2—C10	117.79 (11)
C12—C13—H13	126.1	C5—O3—C11	117.12 (11)
O1—C1—C2—C7	-160.59 (16)	C16—C17—C18—C19	0.8 (2)
C8—C1—C2—C7	19.1 (2)	C17—C18—C19—C20	-0.7 (3)
O1—C1—C2—C3	17.8 (2)	C18—C19—C20—C15	-0.1 (2)
C8—C1—C2—C3	-162.53 (13)	C16—C15—C20—C19	0.8 (2)
C7—C2—C3—C4	-0.3 (2)	N1—C15—C20—C19	-177.60 (14)
C1—C2—C3—C4	-178.78 (12)	N2—C14—C21—C26	39.32 (19)
C2—C3—C4—O2	-179.35 (12)	C12—C14—C21—C26	-143.64 (14)
C2—C3—C4—C5	1.0 (2)	N2—C14—C21—C22	-137.32 (14)
O2—C4—C5—O3	0.76 (17)	C12—C14—C21—C22	39.7 (2)
C3—C4—C5—O3	-179.53 (12)	C26—C21—C22—C23	-0.7 (2)
O2—C4—C5—C6	179.67 (13)	C14—C21—C22—C23	176.01 (13)
C3—C4—C5—C6	-0.6 (2)	C21—C22—C23—C24	0.2 (2)
O3—C5—C6—C7	178.41 (14)	C22—C23—C24—C25	0.2 (2)
C4—C5—C6—C7	-0.4 (2)	C23—C24—C25—C26	0.0 (2)
C3—C2—C7—C6	-0.7 (2)	C24—C25—C26—C21	-0.5 (2)
C1—C2—C7—C6	177.69 (14)	C22—C21—C26—C25	0.8 (2)
C5—C6—C7—C2	1.1 (2)	C14—C21—C26—C25	-175.86 (13)
O1—C1—C8—C9	17.3 (2)	C12—C13—N1—N2	0.22 (16)
C2—C1—C8—C9	-162.38 (14)	C12—C13—N1—C15	-176.70 (13)
C1—C8—C9—C12	-177.91 (13)	C16—C15—N1—C13	21.0 (2)
C8—C9—C12—C13	28.4 (2)	C20—C15—N1—C13	-160.54 (14)
C8—C9—C12—C14	-154.16 (15)	C16—C15—N1—N2	-155.67 (12)
C14—C12—C13—N1	0.05 (15)	C20—C15—N1—N2	22.77 (19)

C9—C12—C13—N1	178.01 (13)	C12—C14—N2—N1	0.43 (15)
C13—C12—C14—N2	-0.31 (16)	C21—C14—N2—N1	177.95 (11)
C9—C12—C14—N2	-178.22 (13)	C13—N1—N2—C14	-0.40 (15)
C13—C12—C14—C21	-177.54 (13)	C15—N1—N2—C14	176.77 (12)
C9—C12—C14—C21	4.5 (2)	C3—C4—O2—C10	6.1 (2)
C20—C15—C16—C17	-0.7 (2)	C5—C4—O2—C10	-174.22 (14)
N1—C15—C16—C17	177.73 (13)	C6—C5—O3—C11	-7.3 (2)
C15—C16—C17—C18	-0.2 (2)	C4—C5—O3—C11	171.50 (14)

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>
C13—H13 \cdots O2 ⁱ	0.94	2.34	3.2648 (19)	169

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