Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-[(*E*)-3-(4-Methoxyphenyl)prop-2-enoyl]-1-(4-methylphenyl)-5-phenyl-1*H*-pyrazole-4-carbonitrile

Hatem A. Abdel-Aziz,[a] Ahmed Bari[a] and Seik Weng Ng[b]*

[a]Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

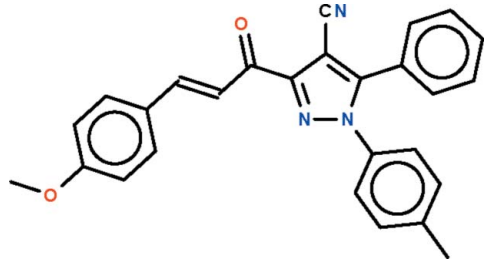
Received 14 February 2011; accepted 16 February 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.133; data-to-parameter ratio = 16.4.

In the title compound, $C_{27}H_{21}N_3O_2$, the non-H atoms of the methoxyphenylacryloyl substitutent of the pyrazolyl ring are almost co-planar (r.m.s. deviation = 0.070 Å), and the mean plane is twisted by 18.7 (1)° with respect to the pyrazolyl ring. The phenyl and tolyl substituents are aligned at 48.9 (1) and 44.5 (1)° with respect to the pyrazolyl ring. Weak intermolecular C—H···O and C—H···N hydrogen bonding is present in the crystal structure.

Related literature

For background to the biological properties of aryl-substituted pyrazoles, see: Abdel-Aziz *et al.* (2010, 2011).



Experimental

Crystal data

$C_{27}H_{21}N_3O_2$
M_r = 419.47
Triclinic, $P\overline{1}$
a = 10.9995 (7) Å
b = 11.0531 (8) Å
c = 11.4381 (8) Å
α = 95.113 (6)°
β = 111.582 (6)°
γ = 118.219 (7)°
V = 1079.13 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.20 × 0.15 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.984, T_{max} = 0.996
8250 measured reflections
4779 independent reflections
3346 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.133
S = 1.05
4779 reflections
291 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.95	2.59	3.350 (3)	137
C22—H22···N3^{ii}	0.95	2.61	3.487 (3)	154
C25—H25···O2^{iii}	0.95	2.56	3.484 (3)	164

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Saud University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5162).

References

Abdel-Aziz, H. A., El-Zahabi, H. S. A. & Dawood, K. M. (2010). *Eur. J. Med. Chem.* **45**, 2427–2432.
Abdel-Aziz, H. A., Nassar, E., Ibrahim, H. S. & Mansour, A. M. (2011). *Bioorg. Med. Chem.* Submitted.
Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, o694 [doi:10.1107/S1600536811005770]

3-[(*E*)-3-(4-Methoxyphenyl)prop-2-enoyl]-1-(4-methylphenyl)-5-phenyl-1*H*-pyrazole-4-carbonitrile

Hatem A. Abdel-Aziz, Ahmed Bari and Seik Weng Ng

S1. Comment

We have reported the antitumor activity of aryl-pyrazoles against CaCo-2 and HEP-2 cell lines (Abdel-Aziz *et al.*, 2010). Among these is the title compound (Scheme I), whose biological properties will be reported elsewhere (Abdel-Aziz *et al.*, 2011). The compound has methoxyphenylacryloyl, phenyl and tolyl substituents in the pyrazolyl ring. The methoxyphenylacryloyl substituent is twisted by 18.7 (1)° with respect to the pyrazolyl ring; the phenyl and tolyl substituents are aligned at 48.9 (1)° and 44.5 (1)° with respect to the five-membered ring (Fig. 1).

S2. Experimental

The synthesis will be reported elsewhere (Abdel-Aziz *et al.*, 2011). 3-Acetyl-5-phenyl-1-*p*-tolyl-1*H*-pyrazole-4-carbonitrile (10 mmol) was reacted with 4-methoxybenzaldehyde (10 mmol) in presence of sodium ethoxide solution (prepared by dissolving 0.23 g sodium metal in 50 ml absolute ethanol). The compound was recrystallized from an ethanol-DMF (3:1) mixture.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

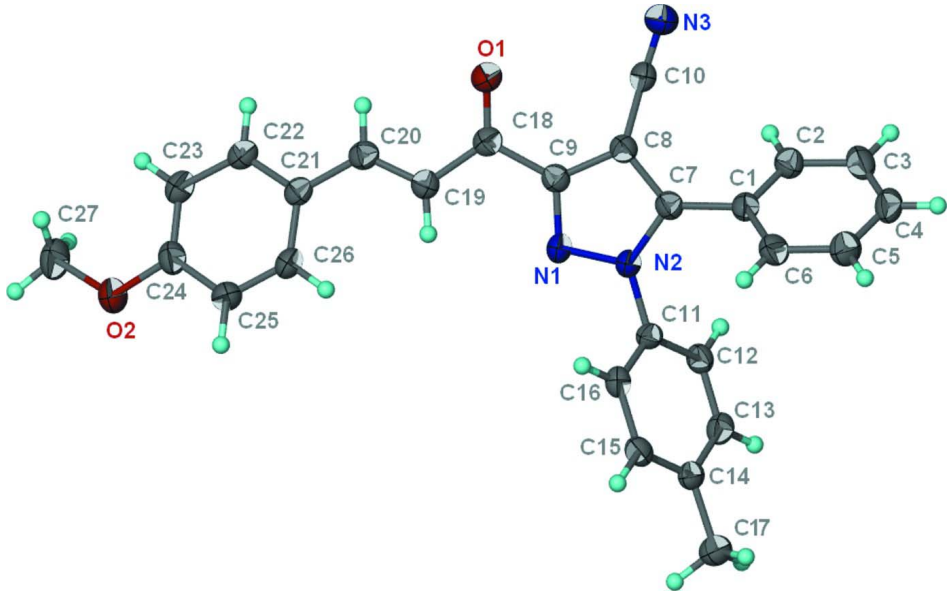


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{27}H_{21}N_3O_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

3-[(*E*)-3-(4-Methoxyphenyl)prop-2-enoyl]-1-(4-methylphenyl)-5- phenyl-1*H*-pyrazole-4-carbonitrile

Crystal data

$C_{27}H_{21}N_3O_2$
$M_r = 419.47$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.9995$ (7) Å
$b = 11.0531$ (8) Å
$c = 11.4381$ (8) Å
$\alpha = 95.113$ (6)°
$\beta = 111.582$ (6)°
$\gamma = 118.219$ (7)°
$V = 1079.13$ (18) Å^3

$Z = 2$
$F(000) = 440$
$D_x = 1.291$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2764 reflections
$\theta = 2.2$–$29.3°$
$\mu = 0.08$ mm^{-1}
$T = 100$ K
Prism, colorless
0.20 × 0.15 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)

$T_{min} = 0.984$, $T_{max} = 0.996$
8250 measured reflections
4779 independent reflections
3346 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.2°$
$h = -10 \rightarrow 13$
$k = -13 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.133$
$S = 1.05$
4779 reflections
291 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
$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 0.3112P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.38684 (16)	0.57825 (15)	0.44798 (13)	0.0300 (3)
O2	0.12051 (18)	0.40793 (16)	1.05036 (14)	0.0367 (4)
N1	0.23698 (18)	0.80105 (17)	0.43686 (15)	0.0234 (4)
N2	0.24257 (18)	0.88927 (17)	0.36089 (15)	0.0224 (4)
N3	0.5147 (2)	0.73362 (19)	0.22677 (18)	0.0346 (4)
C1	0.3312 (2)	0.9656 (2)	0.19190 (18)	0.0240 (4)
C2	0.4740 (2)	1.0450 (2)	0.1918 (2)	0.0279 (4)
H2	0.5633	1.0516	0.2562	0.033*
C3	0.4859 (3)	1.1146 (2)	0.0974 (2)	0.0333 (5)
H3	0.5835	1.1689	0.0975	0.040*
C4	0.3566 (3)	1.1051 (2)	0.0037 (2)	0.0345 (5)
H4	0.3654	1.1535	−0.0602	0.041*
C5	0.2142 (3)	1.0253 (2)	0.0027 (2)	0.0351 (5)
H5	0.1252	1.0183	−0.0626	0.042*
C6	0.2004 (2)	0.9555 (2)	0.09631 (19)	0.0296 (5)
H6	0.1024	0.9011	0.0954	0.036*
C7	0.3174 (2)	0.8880 (2)	0.28932 (18)	0.0232 (4)
C8	0.3647 (2)	0.7940 (2)	0.32243 (18)	0.0231 (4)
C9	0.3105 (2)	0.7419 (2)	0.41342 (18)	0.0230 (4)
C10	0.4468 (2)	0.7579 (2)	0.26995 (19)	0.0253 (4)
C11	0.1709 (2)	0.9692 (2)	0.36361 (17)	0.0219 (4)
C12	0.2558 (2)	1.1174 (2)	0.39088 (18)	0.0242 (4)
H12	0.3621	1.1678	0.4095	0.029*
C13	0.1838 (2)	1.1919 (2)	0.39070 (18)	0.0258 (4)
H13	0.2418	1.2942	0.4103	0.031*
C14	0.0275 (2)	1.1190 (2)	0.36219 (18)	0.0237 (4)
C15	−0.0541 (2)	0.9696 (2)	0.33824 (18)	0.0254 (4)
H15	−0.1599	0.9188	0.3211	0.031*
C16	0.0174 (2)	0.8946 (2)	0.33918 (17)	0.0235 (4)
H16	−0.0386	0.7929	0.3232	0.028*
C17	−0.0532 (3)	1.1984 (2)	0.3558 (2)	0.0328 (5)
H17A	0.0250	1.3027	0.3984	0.049*
H17B	−0.1163	1.1647	0.4020	0.049*
H17C	−0.1209	1.1796	0.2627	0.049*

C18	0.3238 (2)	0.6344 (2)	0.47637 (18)	0.0238 (4)
C19	0.2638 (2)	0.6043 (2)	0.57209 (19)	0.0258 (4)
H19	0.1994	0.6368	0.5774	0.031*
C20	0.2979 (2)	0.5315 (2)	0.65250 (18)	0.0250 (4)
H20	0.3597	0.4983	0.6416	0.030*
C21	0.2506 (2)	0.4980 (2)	0.75476 (18)	0.0235 (4)
C22	0.3173 (2)	0.4435 (2)	0.84454 (19)	0.0259 (4)
H22	0.3919	0.4272	0.8368	0.031*
C23	0.2780 (2)	0.4123 (2)	0.94527 (19)	0.0274 (4)
H23	0.3254	0.3755	1.0058	0.033*
C24	0.1695 (2)	0.4353 (2)	0.95637 (19)	0.0285 (5)
C25	0.0980 (2)	0.4876 (2)	0.8662 (2)	0.0309 (5)
H25	0.0217	0.5016	0.8729	0.037*
C26	0.1392 (2)	0.5187 (2)	0.7676 (2)	0.0280 (4)
H26	0.0911	0.5550	0.7069	0.034*
C27	0.1885 (3)	0.3532 (3)	1.1453 (2)	0.0384 (5)
H27A	0.1401	0.3340	1.2040	0.058*
H27B	0.3008	0.4251	1.1981	0.058*
H27C	0.1710	0.2632	1.0988	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0359 (8)	0.0295 (8)	0.0345 (8)	0.0213 (7)	0.0202 (7)	0.0137 (7)
O2	0.0487 (10)	0.0439 (9)	0.0351 (8)	0.0303 (8)	0.0269 (8)	0.0228 (8)
N1	0.0264 (9)	0.0237 (8)	0.0233 (8)	0.0147 (8)	0.0126 (7)	0.0115 (7)
N2	0.0256 (9)	0.0241 (8)	0.0229 (8)	0.0154 (8)	0.0130 (7)	0.0111 (7)
N3	0.0394 (11)	0.0351 (10)	0.0423 (11)	0.0239 (9)	0.0255 (9)	0.0159 (9)
C1	0.0312 (11)	0.0218 (10)	0.0229 (10)	0.0155 (9)	0.0147 (9)	0.0080 (8)
C2	0.0316 (11)	0.0246 (10)	0.0310 (11)	0.0152 (9)	0.0178 (9)	0.0103 (9)
C3	0.0456 (13)	0.0264 (11)	0.0382 (12)	0.0187 (11)	0.0295 (11)	0.0137 (10)
C4	0.0575 (15)	0.0328 (12)	0.0295 (11)	0.0293 (12)	0.0278 (11)	0.0166 (10)
C5	0.0473 (14)	0.0437 (13)	0.0271 (11)	0.0306 (12)	0.0201 (10)	0.0170 (10)
C6	0.0328 (11)	0.0357 (12)	0.0274 (10)	0.0208 (10)	0.0170 (9)	0.0135 (10)
C7	0.0232 (10)	0.0252 (10)	0.0221 (9)	0.0132 (9)	0.0112 (8)	0.0080 (8)
C8	0.0227 (10)	0.0243 (10)	0.0236 (10)	0.0129 (9)	0.0116 (8)	0.0087 (8)
C9	0.0214 (10)	0.0238 (10)	0.0227 (10)	0.0118 (9)	0.0102 (8)	0.0070 (8)
C10	0.0283 (11)	0.0235 (10)	0.0289 (10)	0.0149 (9)	0.0159 (9)	0.0125 (9)
C11	0.0254 (10)	0.0271 (10)	0.0196 (9)	0.0179 (9)	0.0112 (8)	0.0099 (8)
C12	0.0213 (10)	0.0260 (10)	0.0255 (10)	0.0117 (9)	0.0122 (8)	0.0106 (9)
C13	0.0314 (11)	0.0242 (10)	0.0223 (10)	0.0155 (9)	0.0122 (9)	0.0089 (9)
C14	0.0302 (11)	0.0295 (11)	0.0186 (9)	0.0198 (9)	0.0127 (8)	0.0111 (8)
C15	0.0226 (10)	0.0335 (11)	0.0233 (10)	0.0160 (9)	0.0120 (8)	0.0123 (9)
C16	0.0252 (10)	0.0224 (10)	0.0218 (9)	0.0116 (9)	0.0113 (8)	0.0091 (8)
C17	0.0401 (13)	0.0365 (12)	0.0334 (11)	0.0266 (11)	0.0196 (10)	0.0147 (10)
C18	0.0215 (10)	0.0212 (10)	0.0251 (10)	0.0106 (9)	0.0093 (8)	0.0063 (8)
C19	0.0289 (11)	0.0245 (10)	0.0287 (10)	0.0156 (9)	0.0161 (9)	0.0108 (9)
C20	0.0250 (10)	0.0223 (10)	0.0267 (10)	0.0129 (9)	0.0114 (9)	0.0065 (9)

C21	0.0242 (10)	0.0197 (9)	0.0255 (10)	0.0120 (9)	0.0106 (8)	0.0072 (8)
C22	0.0254 (10)	0.0233 (10)	0.0291 (10)	0.0145 (9)	0.0111 (9)	0.0087 (9)
C23	0.0271 (11)	0.0253 (10)	0.0266 (10)	0.0145 (9)	0.0088 (9)	0.0098 (9)
C24	0.0341 (12)	0.0273 (11)	0.0258 (10)	0.0158 (10)	0.0164 (9)	0.0111 (9)
C25	0.0345 (12)	0.0343 (12)	0.0380 (12)	0.0236 (10)	0.0220 (10)	0.0181 (10)
C26	0.0334 (11)	0.0284 (11)	0.0308 (11)	0.0207 (10)	0.0164 (9)	0.0158 (9)
C27	0.0477 (14)	0.0395 (13)	0.0306 (11)	0.0243 (12)	0.0184 (11)	0.0185 (11)

Geometric parameters (Å, º)

O1—C18	1.228 (2)	C13—C14	1.393 (3)
O2—C24	1.367 (2)	C13—H13	0.9500
O2—C27	1.432 (2)	C14—C15	1.394 (3)
N1—C9	1.335 (2)	C14—C17	1.505 (3)
N1—N2	1.358 (2)	C15—C16	1.386 (3)
N2—C7	1.361 (2)	C15—H15	0.9500
N2—C11	1.440 (2)	C16—H16	0.9500
N3—C10	1.146 (2)	C17—H17A	0.9800
C1—C2	1.391 (3)	C17—H17B	0.9800
C1—C6	1.396 (3)	C17—H17C	0.9800
C1—C7	1.474 (3)	C18—C19	1.461 (3)
C2—C3	1.390 (3)	C19—C20	1.340 (3)
C2—H2	0.9500	C19—H19	0.9500
C3—C4	1.378 (3)	C20—C21	1.456 (3)
C3—H3	0.9500	C20—H20	0.9500
C4—C5	1.382 (3)	C21—C22	1.390 (3)
C4—H4	0.9500	C21—C26	1.402 (3)
C5—C6	1.386 (3)	C22—C23	1.389 (3)
C5—H5	0.9500	C22—H22	0.9500
C6—H6	0.9500	C23—C24	1.378 (3)
C7—C8	1.389 (3)	C23—H23	0.9500
C8—C9	1.417 (3)	C24—C25	1.399 (3)
C8—C10	1.425 (3)	C25—C26	1.376 (3)
C9—C18	1.481 (3)	C25—H25	0.9500
C11—C12	1.379 (3)	C26—H26	0.9500
C11—C16	1.380 (3)	C27—H27A	0.9800
C12—C13	1.387 (3)	C27—H27B	0.9800
C12—H12	0.9500	C27—H27C	0.9800
C24—O2—C27	117.63 (16)	C16—C15—C14	120.69 (18)
C9—N1—N2	105.08 (14)	C16—C15—H15	119.7
N1—N2—C7	112.95 (14)	C14—C15—H15	119.7
N1—N2—C11	118.61 (14)	C11—C16—C15	119.32 (18)
C7—N2—C11	128.44 (15)	C11—C16—H16	120.3
C2—C1—C6	119.62 (18)	C15—C16—H16	120.3
C2—C1—C7	119.97 (17)	C14—C17—H17A	109.5
C6—C1—C7	120.36 (18)	C14—C17—H17B	109.5
C3—C2—C1	119.9 (2)	H17A—C17—H17B	109.5

C3—C2—H2	120.0	C14—C17—H17C	109.5
C1—C2—H2	120.0	H17A—C17—H17C	109.5
C4—C3—C2	120.2 (2)	H17B—C17—H17C	109.5
C4—C3—H3	119.9	O1—C18—C19	123.83 (18)
C2—C3—H3	119.9	O1—C18—C9	118.84 (17)
C5—C4—C3	120.02 (19)	C19—C18—C9	117.31 (16)
C5—C4—H4	120.0	C20—C19—C18	121.14 (18)
C3—C4—H4	120.0	C20—C19—H19	119.4
C4—C5—C6	120.5 (2)	C18—C19—H19	119.4
C4—C5—H5	119.8	C19—C20—C21	127.01 (18)
C6—C5—H5	119.8	C19—C20—H20	116.5
C5—C6—C1	119.7 (2)	C21—C20—H20	116.5
C5—C6—H6	120.1	C22—C21—C26	117.69 (18)
C1—C6—H6	120.1	C22—C21—C20	119.60 (17)
N2—C7—C8	105.58 (16)	C26—C21—C20	122.71 (17)
N2—C7—C1	124.52 (16)	C21—C22—C23	121.73 (18)
C8—C7—C1	129.79 (17)	C21—C22—H22	119.1
C7—C8—C9	105.63 (16)	C23—C22—H22	119.1
C7—C8—C10	125.37 (17)	C24—C23—C22	119.28 (18)
C9—C8—C10	128.98 (17)	C24—C23—H23	120.4
N1—C9—C8	110.75 (16)	C22—C23—H23	120.4
N1—C9—C18	120.93 (16)	O2—C24—C23	124.75 (18)
C8—C9—C18	128.29 (17)	O2—C24—C25	114.80 (18)
N3—C10—C8	177.4 (2)	C23—C24—C25	120.44 (18)
C12—C11—C16	121.29 (17)	C26—C25—C24	119.41 (19)
C12—C11—N2	119.98 (17)	C26—C25—H25	120.3
C16—C11—N2	118.73 (17)	C24—C25—H25	120.3
C11—C12—C13	119.05 (18)	C25—C26—C21	121.43 (18)
C11—C12—H12	120.5	C25—C26—H26	119.3
C13—C12—H12	120.5	C21—C26—H26	119.3
C12—C13—C14	120.95 (18)	O2—C27—H27A	109.5
C12—C13—H13	119.5	O2—C27—H27B	109.5
C14—C13—H13	119.5	H27A—C27—H27B	109.5
C13—C14—C15	118.65 (17)	O2—C27—H27C	109.5
C13—C14—C17	121.14 (18)	H27A—C27—H27C	109.5
C15—C14—C17	120.21 (18)	H27B—C27—H27C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1^{i}	0.95	2.59	3.350 (3)	137
C22—H22···N3^{ii}	0.95	2.61	3.487 (3)	154
C25—H25···O2^{iii}	0.95	2.56	3.484 (3)	164

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