

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

# N-Acetyl-N-[2,4-dicyano-1-(4-methoxyphenyl)-9,10-dihydrophenanthren-3-yl]-acetamide

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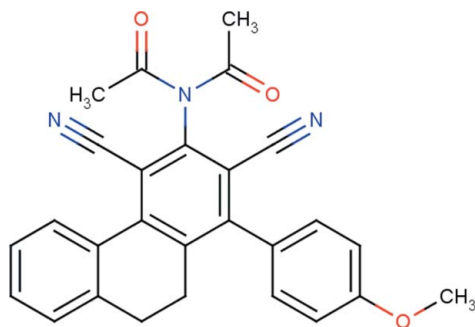
Received 18 March 2012; accepted 21 March 2012

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å; R factor = 0.061;  $wR$  factor = 0.166; data-to-parameter ratio = 17.0.

In the title compound,  $\text{C}_{27}\text{H}_{21}\text{N}_3\text{O}_3$ , the cyclohexa-1,3-diene ring has a screw-boat conformation, and the fused ring system is folded, the dihedral angle between the outer benzene rings being  $27.61(6)^\circ$ . The *N*-acetylacetamide residue (r.m.s. deviation =  $0.0935$  Å) has an *anti* conformation and is essentially perpendicular to the benzene ring to which it is connected [dihedral angle =  $89.14(6)^\circ$ ]; the methoxybenzene group is also twisted out of this ring [dihedral angle =  $59.47(7)^\circ$ ]. The three-dimensional architecture is consolidated by  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\pi$  interactions.

## Related literature

For background to the biological activity of related phenanthrene compounds, see: Wang *et al.* (2010); Rostom *et al.* (2011). For related structures, see: Asiri *et al.* (2011); Al-Youbi *et al.* (2012). For additional conformational analysis, see: Cremer & Pople (1975).


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## Experimental

## Crystal data

$\text{C}_{27}\text{H}_{21}\text{N}_3\text{O}_3$   
 $M_r = 435.47$   
 Orthorhombic, *Pbca*  
 $a = 8.3321(4)$  Å  
 $b = 19.4037(11)$  Å  
 $c = 27.5887(14)$  Å  
 $V = 4460.4(4)$  Å<sup>3</sup>  
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.40 \times 0.20 \times 0.10$  mm

## Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector  
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)  
 $T_{\min} = 0.966$ ,  $T_{\max} = 0.991$   
 11528 measured reflections  
 5106 independent reflections  
 3488 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.041$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$   
 $wR(F^2) = 0.166$   
 $S = 1.02$   
 5106 reflections  
 300 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.39$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.29$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C4–C9 and C21–C26 rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C5}-\text{H5}\cdots\text{O2}^{\text{i}}$	0.95	2.40	3.255 (3)	150
$\text{C25}-\text{H25}\cdots\text{O2}^{\text{ii}}$	0.95	2.59	3.154 (3)	119
$\text{C26}-\text{H26}\cdots\text{O2}^{\text{ii}}$	0.95	2.54	3.141 (3)	121
$\text{C27}-\text{H27A}\cdots\text{O1}^{\text{iii}}$	0.98	2.41	3.160 (3)	133
$\text{C3}-\text{H3B}\cdots\text{Cg1}^{\text{iv}}$	0.99	2.74	3.696 (3)	164
$\text{C19}-\text{H19A}\cdots\text{Cg2}^{\text{v}}$	0.98	2.82	3.618 (3)	139

Symmetry codes: (i)  $-x, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $-x - \frac{1}{2}, y - \frac{1}{2}, z$ ; (iii)  $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$ ; (iv)  $x - \frac{1}{2}, y, -z + \frac{1}{2}$ ; (v)  $x, -y - \frac{1}{2}, z - \frac{1}{2}$ .

Data collection: *CrysAlis PRO* (Agilent, 2011); 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) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors are thankful to the Center of Excellence for Advanced Materials Research and the Chemistry Department at King Abdulaziz University for providing the research facilities. We also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR/MOHE/SC/12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5437).

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## supporting information

*Acta Cryst.* (2012). E68, o1177–o1178 [https://doi.org/10.1107/S160053681201210X]

## *N*-Acetyl-*N*-[2,4-dicyano-1-(4-methoxyphenyl)-9,10-dihydrophenanthren-3-yl]acetamide

Abdullah M. Asiri, Hassan M. Faidallah, Shaeel A. Al-Thabaiti, Seik Weng Ng and Edward R. T. Tiekink

### S1. Comment

The biological activity of phenanthrene compounds (Wang *et al.* 2010; Rostom *et al.*, 2011), has motivated structural studies on these systems Asiri *et al.*, 2011; Al-Youbi *et al.*, 2012) and led to the characterization of the title compound, (I).

In (I), Fig. 1, the cyclohexa-1,3-diene ring has a screw-boat conformation as quantified by the following geometric parameters (Cremer & Pople, 1975): puckering parameters  $q_2 = 0.499$  (2) Å and  $q_3 = 0.176$  (2) Å, and amplitudes:  $Q = 0.529$  (2) Å,  $\theta = 70.6$  (2)° and  $\varphi_2 = 91.2$  (3)°. The benzene rings of the 1,2-dihydronaphthalene and methoxybenzene residues form dihedral angles of 27.61 (6) and 59.47 (7)°, respectively, with the central dicyanobenzene ring, indicating a fold in the fused ring system and a twist of the methoxybenzene ring out of the plane of the benzene ring to which it is connected. The *N*-acetylacetamide residue has an *anti* conformation and is essentially planar. The r.m.s. deviation for the seven fitted atoms = 0.0935 Å with maximum deviations of 0.1476 (15) Å for the O2 atom and -0.1378 (15) Å for the C19 atom. This residue is inclined in a perpendicular fashion with respect to the benzene ring to which it is connected, forming a dihedral angle of 89.14 (6)°.

The three-dimensional architecture of (I) is stabilized by C—H···O and C—H··· $\pi$  interactions, Fig. 2 and Table 1. Notably, the O2 atom of the *N*-acetylacetamide, *i.e.* the oxygen atom residue directed away from the rest of the molecule, participates in three C—H···O interactions, Table 1.

### S2. Experimental

A mixture of 3-amino-1-(4-methoxyphenyl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile (0.01 mmol), acetic anhydride (5 ml) and conc. H<sub>2</sub>SO<sub>4</sub> (0.5 ml) was heated over a boiling water bath for 10 min. The solution was cooled, poured onto ice-cold water, treated with 20% NaOH solution till alkaline (pH = 11). The crude solid product was filtered and recrystallized from ethanol. Yield: 68%. *M.pt.*: 455–457 K.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.99 Å,  $U_{\text{iso}}(\text{H}) = 1.2$  to  $1.5U_{\text{eq}}(\text{C})$ ] and were included in the refinement in the riding model approximation.

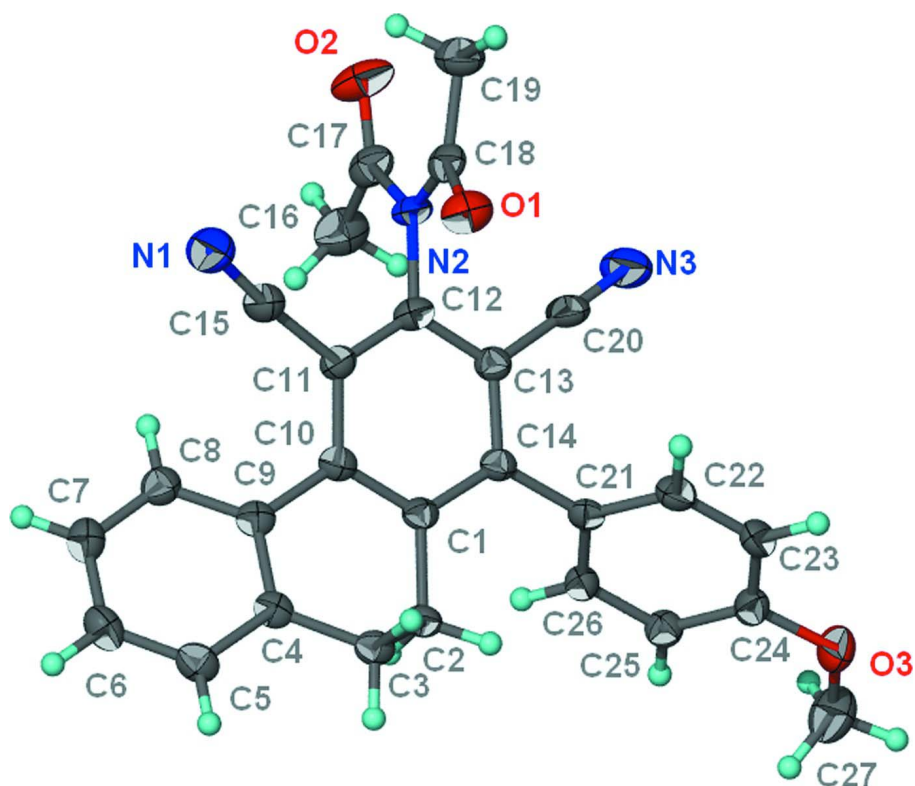
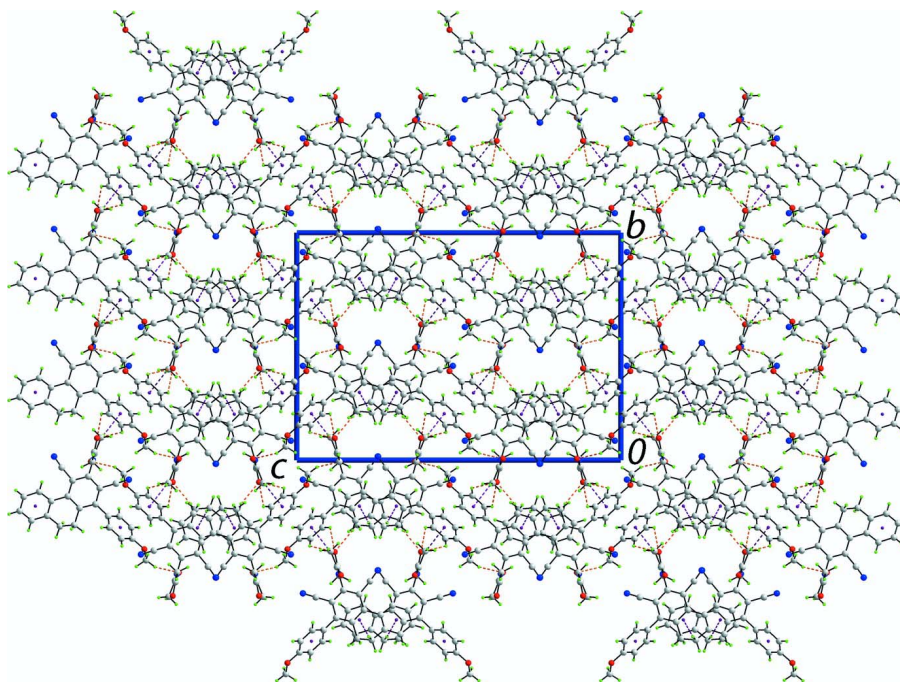


Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.



**Figure 2**

A view in projection down the  $a$  axis of the unit-cell contents of (I). The C—H $\cdots$ O and C—H $\cdots$  $\pi$  interactions are shown as orange and purple dashed lines, respectively.

*N*-Acetyl-*N*-[2,4-dicyano-1-(4-methoxyphenyl)-9,10-dihydrophenanthren-3-yl]acetamide

*Crystal data*

$C_{27}H_{21}N_3O_3$

$M_r = 435.47$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 8.3321$  (4) Å

$b = 19.4037$  (11) Å

$c = 27.5887$  (14) Å

$V = 4460.4$  (4) Å<sup>3</sup>

$Z = 8$

$F(000) = 1824$

$D_x = 1.297$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2867 reflections

$\theta = 2.4$ – $27.5^\circ$

$\mu = 0.09$  mm<sup>-1</sup>

$T = 100$  K

Prism, light-brown

$0.40 \times 0.20 \times 0.10$  mm

*Data collection*

Agilent SuperNova Dual

diffractometer with an Atlas detector

Radiation source: SuperNova (Mo) X-ray

Source

Mirror monochromator

Detector resolution: 10.4041 pixels mm<sup>-1</sup>

$\omega$  scan

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2011)

$T_{\min} = 0.966$ ,  $T_{\max} = 0.991$

11528 measured reflections

5106 independent reflections

3488 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\max} = 27.6^\circ$ ,  $\theta_{\min} = 2.6^\circ$

$h = -10 \rightarrow 7$

$k = -13 \rightarrow 25$

$l = -35 \rightarrow 21$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.061$  $wR(F^2) = 0.166$  $S = 1.02$ 

5106 reflections

300 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 2.7824P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$ *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.2784 (2)	0.49381 (8)	0.63579 (6)	0.0326 (4)
O2	-0.1406 (2)	0.59674 (9)	0.61677 (7)	0.0403 (5)
O3	0.0262 (2)	0.10850 (9)	0.47080 (6)	0.0332 (4)
N1	0.0632 (3)	0.51602 (11)	0.74941 (8)	0.0433 (6)
N2	0.0092 (2)	0.49981 (9)	0.62945 (7)	0.0213 (4)
N3	-0.0310 (3)	0.41448 (11)	0.51859 (8)	0.0392 (6)
C1	0.0157 (2)	0.28935 (11)	0.67074 (8)	0.0189 (5)
C2	0.0293 (3)	0.21508 (11)	0.68718 (8)	0.0210 (5)
H2A	0.0725	0.1866	0.6604	0.025*
H2B	-0.0785	0.1973	0.6956	0.025*
C3	0.1396 (3)	0.20966 (11)	0.73113 (8)	0.0217 (5)
H3A	0.1433	0.1613	0.7426	0.026*
H3B	0.2497	0.2237	0.7220	0.026*
C4	0.0780 (2)	0.25552 (11)	0.77096 (8)	0.0205 (5)
C5	0.0778 (3)	0.23518 (12)	0.81939 (8)	0.0245 (5)
H5	0.1225	0.1918	0.8280	0.029*
C6	0.0133 (3)	0.27708 (13)	0.85540 (8)	0.0273 (5)
H6	0.0167	0.2629	0.8883	0.033*
C7	-0.0557 (3)	0.33955 (13)	0.84298 (8)	0.0269 (5)
H7	-0.1024	0.3677	0.8674	0.032*
C8	-0.0567 (3)	0.36109 (12)	0.79510 (8)	0.0241 (5)
H8	-0.1048	0.4039	0.7869	0.029*
C9	0.0125 (3)	0.32038 (11)	0.75861 (8)	0.0206 (5)
C10	0.0137 (3)	0.34111 (11)	0.70697 (8)	0.0200 (5)
C11	0.0169 (3)	0.41078 (11)	0.69237 (8)	0.0202 (5)
C12	0.0090 (3)	0.42839 (11)	0.64368 (8)	0.0222 (5)
C13	0.0038 (3)	0.37711 (11)	0.60844 (8)	0.0204 (5)
C14	0.0111 (2)	0.30663 (11)	0.62148 (8)	0.0189 (4)
C15	0.0407 (3)	0.46807 (12)	0.72585 (9)	0.0295 (5)
C16	-0.2878 (3)	0.49315 (14)	0.63111 (11)	0.0379 (6)
H16A	-0.3823	0.5230	0.6288	0.057*
H16B	-0.2863	0.4705	0.6629	0.057*
H16C	-0.2922	0.4582	0.6055	0.057*
C17	-0.1384 (3)	0.53571 (12)	0.62517 (9)	0.0288 (5)

C18	0.1648 (3)	0.52930 (12)	0.62423 (8)	0.0247 (5)
C19	0.1828 (3)	0.60013 (12)	0.60405 (9)	0.0336 (6)
H19A	0.2963	0.6091	0.5971	0.050*
H19B	0.1436	0.6338	0.6277	0.050*
H19C	0.1204	0.6040	0.5741	0.050*
C20	-0.0140 (3)	0.39733 (12)	0.55834 (9)	0.0268 (5)
C21	0.0139 (3)	0.25367 (11)	0.58236 (8)	0.0200 (5)
C22	0.1360 (3)	0.25280 (12)	0.54760 (8)	0.0251 (5)
H22	0.2192	0.2862	0.5492	0.030*
C23	0.1380 (3)	0.20432 (12)	0.51101 (8)	0.0266 (5)
H23	0.2224	0.2042	0.4879	0.032*
C24	0.0150 (3)	0.15530 (12)	0.50807 (8)	0.0243 (5)
C25	-0.1080 (3)	0.15542 (11)	0.54194 (8)	0.0223 (5)
H25	-0.1922	0.1226	0.5399	0.027*
C26	-0.1067 (3)	0.20427 (11)	0.57908 (8)	0.0205 (5)
H26	-0.1900	0.2038	0.6026	0.025*
C27	-0.1006 (3)	0.06072 (15)	0.46578 (10)	0.0420 (7)
H27A	-0.0789	0.0304	0.4381	0.063*
H27B	-0.2014	0.0855	0.4603	0.063*
H27C	-0.1093	0.0331	0.4954	0.063*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0286 (9)	0.0278 (9)	0.0413 (10)	-0.0001 (7)	-0.0040 (8)	0.0001 (8)
O2	0.0445 (11)	0.0217 (9)	0.0548 (12)	0.0075 (8)	-0.0187 (9)	-0.0036 (8)
O3	0.0439 (10)	0.0312 (9)	0.0244 (9)	-0.0042 (8)	0.0033 (8)	-0.0079 (7)
N1	0.0689 (17)	0.0307 (12)	0.0303 (11)	-0.0073 (12)	-0.0001 (12)	-0.0032 (10)
N2	0.0276 (10)	0.0130 (9)	0.0234 (9)	0.0005 (7)	-0.0038 (8)	0.0006 (7)
N3	0.0618 (15)	0.0267 (11)	0.0291 (12)	-0.0033 (11)	-0.0083 (11)	0.0036 (9)
C1	0.0163 (10)	0.0169 (11)	0.0235 (11)	-0.0004 (8)	0.0023 (9)	0.0018 (9)
C2	0.0236 (11)	0.0179 (11)	0.0217 (11)	0.0010 (9)	-0.0001 (9)	0.0039 (9)
C3	0.0211 (11)	0.0203 (11)	0.0237 (11)	0.0020 (9)	-0.0015 (9)	0.0035 (9)
C4	0.0156 (10)	0.0226 (11)	0.0232 (11)	-0.0022 (8)	-0.0014 (9)	0.0019 (9)
C5	0.0209 (11)	0.0274 (12)	0.0252 (12)	0.0025 (9)	-0.0028 (9)	0.0064 (10)
C6	0.0261 (12)	0.0351 (14)	0.0208 (11)	-0.0021 (10)	-0.0005 (10)	0.0044 (10)
C7	0.0270 (12)	0.0300 (13)	0.0238 (11)	0.0001 (10)	0.0016 (10)	-0.0025 (10)
C8	0.0230 (11)	0.0227 (12)	0.0267 (12)	-0.0003 (9)	0.0006 (10)	-0.0011 (9)
C9	0.0177 (10)	0.0205 (11)	0.0237 (11)	-0.0018 (9)	-0.0014 (9)	0.0006 (9)
C10	0.0170 (10)	0.0199 (11)	0.0230 (11)	0.0005 (8)	-0.0003 (9)	0.0023 (9)
C11	0.0223 (11)	0.0178 (11)	0.0204 (11)	0.0010 (9)	-0.0012 (9)	-0.0010 (9)
C12	0.0238 (11)	0.0167 (11)	0.0261 (12)	0.0015 (9)	-0.0022 (9)	-0.0001 (9)
C13	0.0226 (11)	0.0190 (11)	0.0196 (10)	-0.0014 (9)	-0.0016 (9)	0.0005 (8)
C14	0.0182 (10)	0.0171 (11)	0.0215 (10)	-0.0010 (8)	0.0009 (9)	0.0015 (9)
C15	0.0393 (14)	0.0232 (12)	0.0259 (12)	-0.0004 (11)	0.0007 (11)	0.0005 (10)
C16	0.0293 (13)	0.0353 (15)	0.0490 (16)	0.0035 (11)	-0.0028 (12)	0.0001 (12)
C17	0.0349 (13)	0.0248 (13)	0.0266 (12)	0.0042 (10)	-0.0079 (11)	-0.0037 (10)
C18	0.0326 (13)	0.0219 (12)	0.0195 (11)	-0.0005 (10)	-0.0038 (10)	-0.0044 (9)



C19	0.0438 (15)	0.0241 (13)	0.0328 (13)	-0.0054 (11)	-0.0042 (12)	0.0029 (10)
C20	0.0372 (13)	0.0158 (11)	0.0273 (12)	-0.0028 (10)	-0.0025 (11)	0.0003 (9)
C21	0.0236 (11)	0.0172 (10)	0.0191 (10)	0.0040 (9)	-0.0006 (9)	0.0045 (8)
C22	0.0266 (12)	0.0220 (12)	0.0269 (12)	-0.0024 (9)	0.0037 (10)	0.0038 (9)
C23	0.0307 (12)	0.0248 (12)	0.0244 (11)	0.0008 (10)	0.0086 (10)	0.0034 (9)
C24	0.0330 (13)	0.0227 (11)	0.0173 (10)	0.0040 (10)	-0.0006 (10)	0.0000 (9)
C25	0.0223 (11)	0.0219 (11)	0.0226 (11)	-0.0016 (9)	-0.0007 (9)	-0.0004 (9)
C26	0.0220 (11)	0.0203 (11)	0.0193 (10)	0.0014 (9)	0.0017 (9)	0.0009 (9)
C27	0.0426 (16)	0.0434 (16)	0.0400 (15)	-0.0022 (13)	-0.0020 (13)	-0.0141 (13)

*Geometric parameters (Å, °)*

O1—C18	1.213 (3)	C10—C11	1.411 (3)
O2—C17	1.207 (3)	C11—C12	1.388 (3)
O3—C24	1.375 (3)	C11—C15	1.459 (3)
O3—C27	1.412 (3)	C12—C13	1.392 (3)
N1—C15	1.150 (3)	C13—C14	1.415 (3)
N2—C17	1.418 (3)	C13—C20	1.445 (3)
N2—C18	1.425 (3)	C14—C21	1.490 (3)
N2—C12	1.440 (3)	C16—C17	1.503 (4)
N3—C20	1.155 (3)	C16—H16A	0.9800
C1—C14	1.400 (3)	C16—H16B	0.9800
C1—C10	1.417 (3)	C16—H16C	0.9800
C1—C2	1.515 (3)	C18—C19	1.490 (3)
C2—C3	1.525 (3)	C19—H19A	0.9800
C2—H2A	0.9900	C19—H19B	0.9800
C2—H2B	0.9900	C19—H19C	0.9800
C3—C4	1.504 (3)	C21—C26	1.392 (3)
C3—H3A	0.9900	C21—C22	1.399 (3)
C3—H3B	0.9900	C22—C23	1.380 (3)
C4—C5	1.393 (3)	C22—H22	0.9500
C4—C9	1.414 (3)	C23—C24	1.400 (3)
C5—C6	1.392 (3)	C23—H23	0.9500
C5—H5	0.9500	C24—C25	1.387 (3)
C6—C7	1.385 (3)	C25—C26	1.396 (3)
C6—H6	0.9500	C25—H25	0.9500
C7—C8	1.385 (3)	C26—H26	0.9500
C7—H7	0.9500	C27—H27A	0.9800
C8—C9	1.403 (3)	C27—H27B	0.9800
C8—H8	0.9500	C27—H27C	0.9800
C9—C10	1.481 (3)		
C24—O3—C27	117.15 (19)	C14—C13—C20	120.66 (19)
C17—N2—C18	125.69 (19)	C1—C14—C13	118.62 (19)
C17—N2—C12	119.62 (19)	C1—C14—C21	122.50 (19)
C18—N2—C12	114.52 (18)	C13—C14—C21	118.87 (19)
C14—C1—C10	120.98 (19)	N1—C15—C11	175.0 (3)
C14—C1—C2	121.35 (19)	C17—C16—H16A	109.5



C10—C1—C2	117.63 (19)	C17—C16—H16B	109.5
C1—C2—C3	110.40 (18)	H16A—C16—H16B	109.5
C1—C2—H2A	109.6	C17—C16—H16C	109.5
C3—C2—H2A	109.6	H16A—C16—H16C	109.5
C1—C2—H2B	109.6	H16B—C16—H16C	109.5
C3—C2—H2B	109.6	O2—C17—N2	120.8 (2)
H2A—C2—H2B	108.1	O2—C17—C16	123.2 (2)
C4—C3—C2	109.55 (17)	N2—C17—C16	116.1 (2)
C4—C3—H3A	109.8	O1—C18—N2	117.1 (2)
C2—C3—H3A	109.8	O1—C18—C19	122.9 (2)
C4—C3—H3B	109.8	N2—C18—C19	120.0 (2)
C2—C3—H3B	109.8	C18—C19—H19A	109.5
H3A—C3—H3B	108.2	C18—C19—H19B	109.5
C5—C4—C9	118.9 (2)	H19A—C19—H19B	109.5
C5—C4—C3	122.2 (2)	C18—C19—H19C	109.5
C9—C4—C3	118.85 (19)	H19A—C19—H19C	109.5
C6—C5—C4	121.3 (2)	H19B—C19—H19C	109.5
C6—C5—H5	119.3	N3—C20—C13	178.5 (3)
C4—C5—H5	119.3	C26—C21—C22	118.2 (2)
C7—C6—C5	119.7 (2)	C26—C21—C14	120.73 (19)
C7—C6—H6	120.2	C22—C21—C14	121.1 (2)
C5—C6—H6	120.2	C23—C22—C21	121.2 (2)
C6—C7—C8	120.2 (2)	C23—C22—H22	119.4
C6—C7—H7	119.9	C21—C22—H22	119.4
C8—C7—H7	119.9	C22—C23—C24	119.8 (2)
C7—C8—C9	120.8 (2)	C22—C23—H23	120.1
C7—C8—H8	119.6	C24—C23—H23	120.1
C9—C8—H8	119.6	O3—C24—C25	123.7 (2)
C8—C9—C4	119.1 (2)	O3—C24—C23	116.3 (2)
C8—C9—C10	122.7 (2)	C25—C24—C23	120.0 (2)
C4—C9—C10	118.10 (19)	C24—C25—C26	119.4 (2)
C11—C10—C1	118.5 (2)	C24—C25—H25	120.3
C11—C10—C9	122.35 (19)	C26—C25—H25	120.3
C1—C10—C9	119.11 (19)	C21—C26—C25	121.4 (2)
C12—C11—C10	120.8 (2)	C21—C26—H26	119.3
C12—C11—C15	115.6 (2)	C25—C26—H26	119.3
C10—C11—C15	123.5 (2)	O3—C27—H27A	109.5
C11—C12—C13	120.1 (2)	O3—C27—H27B	109.5
C11—C12—N2	120.04 (19)	H27A—C27—H27B	109.5
C13—C12—N2	119.8 (2)	O3—C27—H27C	109.5
C12—C13—C14	120.8 (2)	H27A—C27—H27C	109.5
C12—C13—C20	118.5 (2)	H27B—C27—H27C	109.5
C14—C1—C2—C3	141.1 (2)	C11—C12—C13—C14	-1.8 (3)
C10—C1—C2—C3	-36.6 (3)	N2—C12—C13—C14	177.00 (19)
C1—C2—C3—C4	56.6 (2)	C11—C12—C13—C20	176.4 (2)
C2—C3—C4—C5	139.1 (2)	N2—C12—C13—C20	-4.8 (3)
C2—C3—C4—C9	-38.3 (3)	C10—C1—C14—C13	-0.2 (3)

C9—C4—C5—C6	0.6 (3)	C2—C1—C14—C13	-177.90 (19)
C3—C4—C5—C6	-176.9 (2)	C10—C1—C14—C21	179.67 (19)
C4—C5—C6—C7	1.6 (3)	C2—C1—C14—C21	2.0 (3)
C5—C6—C7—C8	-1.7 (4)	C12—C13—C14—C1	3.1 (3)
C6—C7—C8—C9	-0.3 (3)	C20—C13—C14—C1	-175.0 (2)
C7—C8—C9—C4	2.5 (3)	C12—C13—C14—C21	-176.8 (2)
C7—C8—C9—C10	179.8 (2)	C20—C13—C14—C21	5.0 (3)
C5—C4—C9—C8	-2.6 (3)	C18—N2—C17—O2	-0.6 (3)
C3—C4—C9—C8	174.98 (19)	C12—N2—C17—O2	174.6 (2)
C5—C4—C9—C10	-179.99 (19)	C18—N2—C17—C16	178.7 (2)
C3—C4—C9—C10	-2.4 (3)	C12—N2—C17—C16	-6.1 (3)
C14—C1—C10—C11	-3.8 (3)	C17—N2—C18—O1	169.7 (2)
C2—C1—C10—C11	173.92 (19)	C12—N2—C18—O1	-5.6 (3)
C14—C1—C10—C9	177.67 (19)	C17—N2—C18—C19	-11.9 (3)
C2—C1—C10—C9	-4.6 (3)	C12—N2—C18—C19	172.7 (2)
C8—C9—C10—C11	29.9 (3)	C1—C14—C21—C26	60.5 (3)
C4—C9—C10—C11	-152.8 (2)	C13—C14—C21—C26	-119.5 (2)
C8—C9—C10—C1	-151.6 (2)	C1—C14—C21—C22	-120.4 (2)
C4—C9—C10—C1	25.7 (3)	C13—C14—C21—C22	59.5 (3)
C1—C10—C11—C12	5.2 (3)	C26—C21—C22—C23	-0.2 (3)
C9—C10—C11—C12	-176.4 (2)	C14—C21—C22—C23	-179.3 (2)
C1—C10—C11—C15	-170.0 (2)	C21—C22—C23—C24	0.6 (4)
C9—C10—C11—C15	8.5 (3)	C27—O3—C24—C25	3.7 (3)
C10—C11—C12—C13	-2.4 (3)	C27—O3—C24—C23	-177.0 (2)
C15—C11—C12—C13	173.1 (2)	C22—C23—C24—O3	-179.5 (2)
C10—C11—C12—N2	178.78 (19)	C22—C23—C24—C25	-0.2 (3)
C15—C11—C12—N2	-5.7 (3)	O3—C24—C25—C26	178.6 (2)
C17—N2—C12—C11	-89.7 (3)	C23—C24—C25—C26	-0.7 (3)
C18—N2—C12—C11	86.0 (2)	C22—C21—C26—C25	-0.7 (3)
C17—N2—C12—C13	91.5 (3)	C14—C21—C26—C25	178.4 (2)
C18—N2—C12—C13	-92.8 (2)	C24—C25—C26—C21	1.1 (3)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

Cg1 and Cg2 are the centroids of the C4—C9 and C21—C26 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5 $\cdots$ O2 <sup>i</sup>	0.95	2.40	3.255 (3)	150
C25—H25 $\cdots$ O2 <sup>ii</sup>	0.95	2.59	3.154 (3)	119
C26—H26 $\cdots$ O2 <sup>ii</sup>	0.95	2.54	3.141 (3)	121
C27—H27A $\cdots$ O1 <sup>iii</sup>	0.98	2.41	3.160 (3)	133
C3—H3B $\cdots$ Cg1 <sup>iv</sup>	0.99	2.74	3.696 (3)	164
C19—H19A $\cdots$ Cg2 <sup>v</sup>	0.98	2.82	3.618 (3)	139

Symmetry codes: (i)  $-x, y-1/2, -z+3/2$ ; (ii)  $-x-1/2, y-1/2, z$ ; (iii)  $x-1/2, -y+1/2, -z+1$ ; (iv)  $x-1/2, y, -z+1/2$ ; (v)  $x, -y-1/2, z-1/2$ .