organic compounds

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5-Acetyl-4-(2-chlorophenyl)-6-methyl-3,4-dihydropyrimidin-2(1H)-one

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.090; data-to-parameter ratio = 21.1.

In the title molecule, $C_{13}H_{13}CIN_2O_2$, the heterocyclic ring adopts a flattened boat conformation with the plane through the four coplanar atoms making a dihedral angle of $89.16 (5)^{\circ}$ with the benzene ring, which adopts an axial orientation. The carbonyl, acetyl and methyl groups each have an equatorial orientation. In the crystal structure, intermolecular $N-H \cdots O$ hydrogen bonds lead to a tape motif. The H atoms of the methyl group at position 6 are disordered over two positions of opposite orientation.

Related literature

For the biological applications of dihydropyrimidinone derivatives, see: Ghorab et al. (2000); Kappe (1993, 2000); Kappe et al. (1997); Rovnyak et al. (1992, 1995); Shivarama Holla et al. (2004).



Experimental

Crystal data C13H13ClN2O2 $M_r = 264.70$ Orthorhombic, Pna21 a = 14.5364 (8) Å b = 12.1587 (5) Å c = 7.0780 (4) Å

 $V = 1250.99 (11) \text{ Å}^3$ Z = 4Mo $K\alpha$ radiation $\mu = 0.30 \text{ mm}^{-1}$ T = 296 (2) K $0.58\,\times\,0.22\,\times\,0.16$ mm

Data collection

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Bruker APEXII CCD
  diffractometer
Absorption correction: multi-scan
  (SADABS; Bruker, 2004)
  T_{\rm min} = 0.845, T_{\rm max} = 0.954
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Refinement

R[wl S

36 17

11

$F^2 > 2\sigma(F^2)$] = 0.037	H atoms treate
$R(F^2) = 0.090$	independent
= 1.03	refinement
37 reflections	$\Delta \rho_{\rm max} = 0.20 \ {\rm e}$
2 parameters	$\Delta \rho_{\min} = -0.22$
restraint	Absolute struct
	1654 Friedel

3637 independent reflections 3087 reflections with $I > 2\sigma(I)$ $R_{\rm int} = 0.043$

22043 measured reflections

H atoms treated by a mixture of independent and constrained
and point and constrained
refinement
$\Delta \rho_{\rm max} = 0.20 \text{ e } \text{\AA}^{-3}$
$\Delta \rho_{\rm min} = -0.22 \text{ e } \text{\AA}^{-3}$
Absolute structure: Flack (1983),
1654 Friedel pairs
Flack parameter: 0.01 (6)

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

$D - H \cdots A$	D-H	$H \cdots A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$\begin{array}{l} N1 - H1 \cdots O2^{i} \\ N3 - H3 \cdots Cl1 \\ N3 - H3 \cdots O2^{ii} \\ C4 - H4 \cdots O15 \\ C16 - H16A \cdots O2^{iii} \\ C45 - H45 \cdots O15^{iv} \\ C16 - H16C \cdots Cg^{iii} \end{array}$	0.80 (2) 0.83 (2) 0.83 (2) 0.98 0.96 0.93 0.96	2.05 (2) 2.748 (18) 2.18 (2) 2.35 2.51 2.55 2.86	2.8386 (18) 3.2005 (15) 2.9627 (18) 2.712 (2) 3.421 (2) 3.257 (3) 3.699 (2)	170.6 (19) 116.2 (14) 158.6 (16) 101 159 133 147

Symmetry codes: (i) $-x + 1, -y + 1, z - \frac{1}{2}$; (ii) $-x + 1, -y + 1, z + \frac{1}{2}$; (iii) $x - \frac{1}{2}, -y + \frac{1}{2}, z$; (iv) $-x + 1, -y, z - \frac{1}{2}$. Cg is the centroid of the C41–C46 ring

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2; data reduction: SAINT-NT (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2333).

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supplementary materials

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5-Acetyl-4-(2-chlorophenyl)-6-methyl-3,4-dihydropyrimidin-2(1H)-one

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Comment

Dihydropyrimidinone derivatives exhibit a wide range of biological effects including anti-fungal, anti-viral, anti-cancer, anti-bacterial, and anti-inflammatory activities (Kappe, 2000; Ghorab *et al.*, 2000; Shivarama Holla *et al.*, 2004). Some dihydropyrimidinones exhibit anti-tumour properties (Kappe, 1993). In addition, these compounds have emerged as the integral backbones of several calcium channel blockers (Rovnyak *et al.*, 1995), antagonists (Kappe *et al.*, 1997) and anti-hypertensive agents (Rovnyak *et al.*, 1992).

In the title molecule, $C_{13}H_{13}ClN_2O_2$, (I) & Fig. 1, the heterocyclic ring adopts a flattened boat conformation with the plane through the four co- planar atoms (N3, C2, C5 and C6) forming a dihedral angle of 89.16 (5)° with the benzene ring, which is in an axial orientation. The carbonyl, acetyl and methyl groups are each in an equatorial orientation. Intermolecular N1—H1···O2, N3—H3···O2, C16—H16A···O2 and C45—H45···O15 interactions, and N3—H3···Cl1 and C4—H4···O15 intramolecular contacts are found, Table 1. The N—H···O hydrogen bonding leads to the formation of tapes. Further, a C16—H16C··· π interaction is also found involving the benzene (C41—C46) ring. Fig. 2 shows a view of the unit-cell contents.

Experimental

A solution of acetylacetone (1.0012 g, 0.01 mol), 2-chlorobenzaldehyde (1.4057 g, 0.01 mol) and urea (0.90 g, 0.015 mol) was heated under reflux in the presence of calcium chloride (0.1109 g, 0.001 mol) for 5 h (monitored by TLC). After completion of the reaction, the reaction mixture was cooled to room temperature and poured into crushed ice. The solid product was filtered under suction and purified by column chromatography on silica gel. Elution with 1:1 (benzene:ethyl acetate v/v) gave the product in the pure form. Yield 0.79 g (88%).

Refinement

The N-bound H atoms were located in a difference Fourier map and refined isotropically, see Table 1 for bond distances. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 - 0.98 Å and $U_{iso}(H) = 1.2 - 1.5$ times $U_{eq}(C)$. The H atoms bound to the C6-methyl group were found to be disordered over two positions with equal weight.

Figures



Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius.



5-Acetyl-4-(2-chlorophenyl)-6-methyl-3,4-dihydropyrimidin-2(1H)-one

Crystal data

$D_{\rm x} = 1.406 {\rm ~Mg~m}^{-3}$
Melting point: 555.5 K
Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Cell parameters from 6857 reflections
$\theta = 2.8 - 25.4^{\circ}$
$\mu = 0.30 \text{ mm}^{-1}$
T = 296 (2) K
Needle, colourless
$0.58\times0.22\times0.16~mm$

Data collection

Bruker APEXII CCD diffractometer	3637 independent reflections
Radiation source: fine-focus sealed tube	3087 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.043$
T = 296(2) K	$\theta_{max} = 30.1^{\circ}$
φ and ω scans	$\theta_{\min} = 2.2^{\circ}$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -20 \rightarrow 20$
$T_{\min} = 0.845, \ T_{\max} = 0.954$	$k = -17 \rightarrow 16$
22043 measured reflections	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.1683P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.090$	$(\Delta/\sigma)_{\rm max} = 0.001$
<i>S</i> = 1.03	$\Delta \rho_{max} = 0.20 \text{ e } \text{\AA}^{-3}$
3637 reflections	$\Delta \rho_{min} = -0.22 \text{ e } \text{\AA}^{-3}$
172 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1654 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.01 (6)

Secondary atom site location: difference Fourier map

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\sigma(F^2)$ 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 (A^2)

	x	У	Z	$U_{\rm iso}$ */ $U_{\rm eq}$	Occ. (<1)
Cl1	0.55079 (4)	0.22136 (5)	1.08117 (7)	0.0597 (2)	
O2	0.50642 (8)	0.51312 (9)	0.62182 (16)	0.0343 (3)	
O15	0.27723 (11)	0.09996 (13)	0.7672 (3)	0.0774 (6)	
N1	0.42438 (10)	0.38746 (11)	0.4557 (2)	0.0317 (4)	
N3	0.44410 (10)	0.36578 (10)	0.7731 (2)	0.0307 (4)	
C2	0.46183 (10)	0.42625 (12)	0.6203 (2)	0.0272 (4)	
C4	0.41461 (11)	0.25076 (12)	0.7555 (2)	0.0287 (4)	
C5	0.34298 (9)	0.24351 (12)	0.6009 (2)	0.0292 (4)	
C6	0.35395 (10)	0.31050 (12)	0.4495 (2)	0.0292 (4)	
C15	0.27134 (12)	0.16018 (14)	0.6294 (3)	0.0411 (5)	
C16	0.19130 (12)	0.14572 (17)	0.4994 (4)	0.0527 (7)	
C41	0.49732 (11)	0.17499 (12)	0.7223 (2)	0.0289 (4)	
C42	0.56389 (12)	0.15910 (13)	0.8612 (3)	0.0375 (5)	
C43	0.64096 (14)	0.09425 (16)	0.8322 (3)	0.0486 (6)	
C44	0.65258 (14)	0.04277 (16)	0.6600 (3)	0.0484 (6)	
C45	0.58767 (13)	0.05448 (15)	0.5208 (3)	0.0430 (5)	

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C46	0.51081 (12)	0.11989 (13)	0.5529 (2)	0.0351 (5)	
C61	0.30143 (13)	0.31541 (15)	0.2672 (3)	0.0423 (5)	
H1	0.4383 (13)	0.4194 (16)	0.362 (3)	0.039 (5)*	
Н3	0.4662 (12)	0.3844 (14)	0.876 (3)	0.028 (5)*	
H4	0.38548	0.22909	0.87471	0.0345*	
H16A	0.15191	0.08874	0.54708	0.0791*	
H16B	0.21307	0.12573	0.37608	0.0791*	
H16C	0.15749	0.21339	0.49164	0.0791*	
H43	0.68435	0.08551	0.92754	0.0584*	
H44	0.70457	0.00002	0.63836	0.0581*	
H45	0.59505	0.01882	0.40558	0.0516*	
H46	0.46706	0.12694	0.45776	0.0421*	
H61A	0.32656	0.37231	0.18861	0.0635*	0.500
H61B	0.23793	0.33107	0.29304	0.0635*	0.500
H61C	0.30619	0.24599	0.20333	0.0635*	0.500
H61D	0.25389	0.26060	0.26804	0.0635*	0.500
H61E	0.34252	0.30185	0.16361	0.0635*	0.500
H61F	0.27426	0.38692	0.25332	0.0635*	0.500

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0743 (3)	0.0725 (3)	0.0323 (2)	0.0214 (3)	-0.0192 (2)	-0.0082 (2)
O2	0.0433 (6)	0.0301 (5)	0.0294 (6)	-0.0071 (4)	-0.0026 (5)	0.0000 (4)
015	0.0606 (9)	0.0728 (10)	0.0989 (14)	-0.0278 (8)	-0.0217 (9)	0.0522 (10)
N1	0.0394 (7)	0.0341 (6)	0.0216 (6)	-0.0083 (5)	-0.0014 (6)	0.0039 (5)
N3	0.0430 (8)	0.0278 (6)	0.0212 (6)	-0.0006 (5)	-0.0028 (6)	-0.0001 (5)
C2	0.0303 (7)	0.0269 (6)	0.0244 (7)	0.0021 (5)	0.0006 (5)	0.0002 (5)
C4	0.0333 (7)	0.0282 (6)	0.0247 (7)	-0.0022 (6)	0.0018 (6)	0.0040 (5)
C5	0.0250 (6)	0.0306 (7)	0.0321 (8)	-0.0014 (5)	0.0002 (6)	0.0029 (6)
C6	0.0276 (7)	0.0312 (7)	0.0289 (8)	0.0005 (6)	-0.0009 (6)	-0.0001 (6)
C15	0.0309 (8)	0.0366 (8)	0.0558 (12)	-0.0015 (6)	-0.0004 (8)	0.0099 (8)
C16	0.0332 (9)	0.0493 (10)	0.0757 (15)	-0.0123 (8)	-0.0068 (9)	0.0098 (10)
C41	0.0307 (8)	0.0268 (6)	0.0292 (8)	-0.0029 (5)	-0.0010 (6)	0.0044 (5)
C42	0.0436 (9)	0.0360 (8)	0.0328 (8)	0.0025 (7)	-0.0059 (7)	0.0011 (7)
C43	0.0448 (10)	0.0489 (10)	0.0522 (11)	0.0116 (8)	-0.0135 (9)	0.0044 (9)
C44	0.0428 (10)	0.0409 (9)	0.0616 (13)	0.0128 (8)	0.0011 (9)	-0.0012 (9)
C45	0.0459 (10)	0.0367 (8)	0.0465 (10)	0.0027 (7)	0.0052 (8)	-0.0087 (7)
C46	0.0381 (8)	0.0338 (7)	0.0334 (9)	-0.0009 (6)	-0.0031 (7)	-0.0031 (6)
C61	0.0423 (9)	0.0493 (10)	0.0354 (8)	-0.0078 (8)	-0.0091 (8)	0.0036 (8)

Geometric parameters (Å, °)

Cl1—C42	1.742 (2)	C43—C44	1.381 (3)
O2—C2	1.2393 (18)	C44—C45	1.372 (3)
O15—C15	1.223 (3)	C45—C46	1.390 (3)
N1—C2	1.370 (2)	C4—H4	0.9800
N1—C6	1.388 (2)	C16—H16A	0.9600
N3—C2	1.333 (2)	C16—H16B	0.9600

N3—C4	1.4680 (19)	C16—H16C	0.9600
N1—H1	0.80 (2)	C43—H43	0.9300
N3—H3	0.83 (2)	C44—H44	0.9300
C4—C41	1.533 (2)	C45—H45	0.9300
C4—C5	1.513 (2)	C46—H46	0.9300
C5—C6	1.355 (2)	C61—H61A	0.9600
C5—C15	1.467 (2)	С61—Н61В	0.9600
C6—C61	1.501 (3)	С61—Н61С	0.9600
C15—C16	1.494 (3)	С61—Н61D	0.9600
C41—C46	1.387 (2)	C61—H61E	0.9600
C41—C42	1.393 (2)	C61—H61F	0.9600
C42—C43	1.385 (3)		
Cl1···N3	3.2005 (15)	C46…H16C ^v	2.9700
Cl1···C46 ⁱ	3.6067 (15)	C61…H16B	2.7500
Cl1···O2 ⁱⁱ	3.3462 (13)	C61…H16C	2.9100
Cl1···H4	2.8100	H1…H61A	2.1100
Cl1···H46 ⁱ	3.1500	H1…H61E	2.4400
Cl1…H3	2.748 (18)	H1…H61F	2.5400
O2…Cl1 ⁱⁱⁱ	3.3462 (13)	H1…O2 ⁱⁱⁱ	2.05 (2)
O2…N1 ⁱⁱ	2.8386 (18)	H1…C2 ⁱⁱⁱ	2.93 (2)
O2…N3 ⁱⁱⁱ	2.9627 (18)	H3…Cl1	2.748 (18)
O15····C45 ^{iv}	3.257 (3)	H3…C42	3.087 (17)
O15…C41	3.342 (2)	H3····O2 ⁱⁱ	2.18 (2)
O2…H61A ⁱⁱ	2.8400	H3····C2 ⁱⁱ	3.064 (19)
O2…H1 ⁱⁱ	2.05 (2)	H4…Cl1	2.8100
O2…H3 ⁱⁱⁱ	2.18 (2)	H4…O15	2.3500
$O2 \cdots H16A^{v}$	2.5100	H4…H61E ⁱ	2.3100
O15…H4	2.3500	H16A…O2 ^{vii}	2.5100
O15····H44 ^{iv}	2.9100	H16A…C2 ^{vii}	2.8200
O15…H45 ^{iv}	2.5500	H16B…C6	3.0800
O15····H61F ^{vi}	2.7000	H16B…C61	2.7500
N1…C41	3.370 (2)	H16B…H61B	2.5900
N1····O2 ⁱⁱⁱ	2.8386 (18)	H16B…H61C	2.3400
N3…Cl1	3.2005 (15)	H16B…H61D	1.9000
N3····O2 ⁱⁱ	2.9627 (18)	H16B…H44 ^{viii}	2.5700
C2…C16 ^v	3.553 (2)	H16C…C61	2.9100
C6…C46	3.333 (2)	H16C…H61B	2.3200
C15…C46	3.557 (2)	H16C…H61D	2.1900
C16…C2 ^{vii}	3.553 (2)	H16C···C45 ^{vii}	3.0100
C16…C61	3.086 (3)	H16C···C46 ^{vii}	2.9700
C41…O15	3.342 (2)	H44…O15 ^{viii}	2.9100
C41…N1	3.370 (2)	H44···H16B ^{iv}	2.5700
C42····C45 ^{iv}	3.588 (3)	H45…O15 ^{viii}	2.5500

supplementary materials

C45- 015^{viii} 3.257 (3)H46- $C11^{ix}$ 3.1500C46- $C1^{1x}$ 3.6067 (15)H46- $C5$ 2.5100C46- $C6$ 3.337 (2)H46- $C6$ 2.7700C46- $C6$ 3.332 (2)H61A- $H11$ 2.1100C1- $C16$ 3.086 (3)H61A- $O2^{ii}$ 2.8400C2- $H16A^x$ 2.8200H61B- $H16C$ 2.3500C2- $H1i^{1i}$ 2.93 (2)H61B- $H16C$ 2.3500C2- $H3^{iii}$ 3.064 (19)H61B- $H16C$ 2.3500C3-H462.5100H61B- $C16$ 2.9400C6- $H46$ 2.7700H61C- $C16$ 2.9400C6- $H461D$ 2.8500H61D- $C15$ 2.8500C16- $H61D$ 2.3400H61D- $H16B$ 2.9000C16- $H61D$ 2.3400H61D- $H16B$ 2.1900C16- $H61B$ 2.7700H61D- $H16C$ 2.1900C41- $H45^{ix}$ 3.0100H61E- $H1$ 2.4400C42- $H3$ 3.087 (17)H61E- $H1$ 2.4400C42- $H3$ 3.0500H61F- $H1$ 2.5400C45- $H161B^{ix}$ 3.0500H61F- $H1$ 2.5400C45- $H161B^{ix}$ 3.0500H61F- $H1$ 2.5400C45- $H111$ 1.92 (12)H61B- $H16C$ 1.9000C2- $N3-C4$ 120.87 (13)C15- $C16-H16B$ 199.00C4- $N3-H41$ 119.20 (12)H61B- $H16C$ 199.00C4- $N3-H41$ 119.20 (12)H61B- $H16C$ 199.00C4- $N3-H43$ 120.00C1- $C-H16B$ 199.00C4- $N3-H43$ 120.00C1- $C2-N3$ 115.57 (13)C45- $C16-H16B$ <t< th=""><th>C45····C42^{viii}</th><th>3.588 (3)</th><th>H45····C41^{viii}</th><th>3.0100</th></t<>	C45····C42 ^{viii}	3.588 (3)	H45····C41 ^{viii}	3.0100
C46-C1Ix $3.6067 (15)$ H46-C5 2.5100 C46-C6 $3.357 (2)$ H46-C6 2.7700 C46-C6 $3.332 (2)$ H61A-H1 2.1100 C46-C6 $3.386 (3)$ H61A-C2 ⁱⁱⁱ 2.8400 C2-H16A ^x 2.8200 H61B-C16 2.7700 C2-H1 ⁱⁱ $2.93 (2)$ H61B-H16B 2.5900 C2-H3 ⁱⁱⁱ $3.064 (19)$ H61B-H16C 2.3200 C5-H46 2.7700 H61C-C16 2.9400 C6-H16B 3.0800 H61C-C16 2.8300 C6-H46 2.7700 H61D-C16 2.8400 C16-H61D 2.8500 H61D-C16 2.9400 C16-H61D 2.3400 H61D-H16C 2.1900 C16-H61B 2.7700 H61D-H16C 2.1900 C16-H61B 2.7700 H61E-H1 2.4400 C42-H13 $3.087 (17)$ H61E-H1 2.4400 C42-H14 3.0500 H61F-H1 2.5400 C45-H161V 3.0500 H61F-H1 2.5400 C45-H161V 3.0500 H61F-H1 2.5400 C45-H161V 3.0500 H61F-H1 2.5400 C4-H14C $1.23.53 (13)$ C15-C16-H16819.000C2-N3-C4 $12.857 (13)$ C15-C16-H16819.000C2-N3-H3 $119.2 (12)$ H16B-C16-H16819.00C4-N3-H3 $119.2 (12)$ H16B-C16-H16819.00C4-N3-H3 $119.2 (12)$ H16B-C16-H16819.00C4-N3-H3 $119.2 (12)$ H16B-C16-H16819.00C4-N3-H3 $119.2 (12)$ C4-C43-H43 </td <td>C45…O15^{viii}</td> <td>3.257 (3)</td> <td>H46…Cl1^{ix}</td> <td>3.1500</td>	C45…O15 ^{viii}	3.257 (3)	H46…Cl1 ^{ix}	3.1500
C46-C15 3.557 (2) H46-C6 2.7700 C46-C6 3.333 (2) H61A-·111 2.1100 C61-C16 3.086 (3) H61A-·02 ⁱⁱⁱ 2.8400 C2H16A ^x 2.8200 H61B-·C16 2.7700 C2H3 ⁱⁱⁱ 2.93 (2) H61B-·H16B 2.3200 C3H46 2.5100 H61B-·C16 2.3200 C6H46 2.7700 H61C-·C16 2.3400 C16-·H61B 3.0800 H61D-·C15 2.8500 C16-·H61D 2.3400 H61D-·H16B 1.9000 C16-·H61D 2.3400 H61D-·H16B 1.9000 C46-·H45 ⁱ 3.0100 H61E-·H1 2.4400 C45-·H161 ^k 3.0500 H61E-·H1 2.4400 C45-·H162 2.9000 C41-·H45 ⁱⁱ 2.3100 C45-·H165 3.0500 H61E-·H1 2.4400 C45-·H162 2.9000 C41-·H45 ⁱⁱ 2.9000 C45-·H165 2.9000 C45-·H165 1.9000 C45-·H	C46····Cl1 ^{ix}	3.6067 (15)	H46…C5	2.5100
C46C6 3.333 (2) H61AH1 2.1100 C61C16 3.086 (3) H61AO2 ^{min} 2.8400 C2H1 ^{min} 2.93 (2) H61BC16 2.7700 C2H3 ^{min} 3.064 (19) H61BH16C 2.3200 C5H46 2.5100 H61BC45 ^{crin} 3.0500 C6H46 2.7700 H61CC16 2.9400 C16H61D 2.8500 H61DC15 2.8500 C16H61D 2.3400 H61DC16 2.3400 C16H61B 2.7700 H61DH16C 2.1900 C41H45 ^{kin} 3.0100 H61EH1 2.4400 C42H3 3.087 (17) H61EH1 2.4000 C42H3 3.087 (17) H61EH1 2.400 C42H3 3.087 (17) H61EH1 2.400 C42H3 3.087 (17) H61EH1 2.400 C42H16H ^{kin} 3.0100 H61FM1 2.400 C2-N3-C4 12.087 (13) C15-C16-H16E 109.00 C2-N3-M2 12.020 (11) <	C46…C15	3.557 (2)	H46…C6	2.7700
C61-C16 3.086 (3) H61A- 02^{iii} 2.8400 C2-H16A ^v 2.8200 H61B-C16 2.7700 C2-H1 ⁱⁱ 2.93 (2) H61B-H16B 2.5900 C2-H14 ⁱⁱⁱ 3.064 (19) H61B-C45 ^{vii} 3.0500 C5-H46 2.5100 H61B-C45 ^{vii} 3.0500 C6-H46 2.7700 H61D-C16 2.9400 C16-H161D 2.8500 H61D-C16 2.3400 C16-H61C 2.9400 H61D-C16 2.3400 C16-H61D 2.3400 H61D-H162 2.1900 C42-H3 3.087 (17) H61E-H4 ^{ax} 2.3100 C42-H3 3.087 (17) H61E-H4 ^{ax} 2.3100 C42-H3 3.087 (13) C15-C16-H16B 199.00 C2-N1-C6 123.53 (13) C15-C16-H16B 199.00 C2-N1-C6 123.53 (13) C15-C16-H16B 199.00 C2-N1-H1 116.1 (4) H16A-C16-H16C 199.00 C2-N3-H3 119.2 (12) H16B-C16-H16C 199.00 C2-N3-H3 116.7 (12)<	C46···C6	3.333 (2)	H61A…H1	2.1100
C2H16A*2.8200H61BC162.7700C2H1i ⁱⁱ 2.93 (2)H61BH16B2.5900C2H3 ⁱⁱⁱ 3.064 (19)H61BC45 ^{vii} 3.0500C5H462.5100H61BC45 ^{vii} 3.0500C6H462.7700H61CC162.9400C6H463.0800H61DC152.8500C16H61D2.8400H61DH16B2.3400C16H61D2.9400H61DH16B1.9000C16H61B2.7700H61DH16B1.9000C16H61B2.7700H61DH16B2.9000C41H45 ^{iv} 3.0100H61EH12.4400C42H33.087 (17)H61EH12.4400C42H61B2.7700H61F015 ⁸ 2.7000C45H61B*3.0100H61F015 ⁸ 2.7000C45H61B*3.0100H61F015 ⁸ 2.7000C2N1-C612.353 (13)C15C16H16B109.00C2N3-C412.087 (13)C15C16H16B109.00C2-N3-C412.087 (13)C15C16H16C100.00C4-N3-H3119.2 (12)H16BC16H16C100.00C2-N3-M3119.2 (12)H16BC16H16C109.00C2-N3-M3119.2 (12)H16BC16H16C109.00C3C410.853 (13)C43C44H44120.00O2-C2-N112.058 (13)C43C44H44120.00O2-C2-N112.058 (13)C43C44H44120.00O3-C4-C5115.43 (13)C45C44H46119.00C4C5-C6117.12 (13)<	C61…C16	3.086 (3)	H61A…O2 ⁱⁱⁱ	2.8400
$\begin{array}{cccccc} C2-H1^{ii} & 2.93 (2) & H61B-H16B & 2.5900 \\ C2-H3^{ii} & 3.064 (19) & H61B-C45^{*ij} & 3.0500 \\ C5-H46 & 2.5100 & H61D-C16 & 2.9400 \\ C6-H16B & 3.0800 & H61C-H16B & 2.3400 \\ C15-H61D & 2.8500 & H61D-C15 & 2.8500 \\ C16-H61D & 2.9400 & H61D-H16B & 1.9000 \\ C16-H61B & 2.7700 & H61D-H16B & 1.9000 \\ C16-H61B & 2.7700 & H61D-H16B & 1.9000 \\ C16-H61B & 2.7700 & H61D-H16B & 1.9000 \\ C42-H3 & 3.0100 & H61E-H1 & 2.4400 \\ C42-H3 & 3.0500 & H61F-H1 & 2.5400 \\ C45-H16C^V & 3.0100 & H61F-H1 & 2.5400 \\ C45-H16C^V & 3.0100 & H61F-H1 & 2.5400 \\ C2-N1-C6 & 123.53 (13) & C15-C16-H16B & 109.00 \\ C2-N3-C4 & 120.87 (13) & C15-C16-H16B & 109.00 \\ C2-N3-C4 & 120.87 (13) & C15-C16-H16B & 109.00 \\ C2-N3-H3 & 119.2 (12) & H16B-C16-H16C & 110.00 \\ C4-N3-H3 & 119.2 (12) & H16B-C16-H16C & 109.00 \\ C2-N3-H3 & 119.2 (12) & H16B-C16-H16C & 109.00 \\ C2-N3-H3 & 119.2 (12) & H6B-C16-H16C & 109.00 \\ C2-N3-H3 & 119.2 (12) & H6B-C16-H16C & 109.00 \\ C2-N3-H3 & 119.2 (12) & H6B-C16-H16C & 109.00 \\ C2-N3-H3 & 115.05 (13) & C43-C44-H44 & 120.00 \\ O2-C2-N3 & 115.05 (13) & C43-C44-H44 & 120.00 \\ O2-C2-N1 & 120.58 (13) & C45-C44-H44 & 120.00 \\ O3-C4-C5 & 108.53 (12) & C44-C45-H45 & 120.00 \\ O3-C4-C41 & 113.20 (12) & C41-C46-H46 & 119.00 \\ C4-C5-C15 & 115.43 (13) & C45-C44-H44 & 120.00 \\ O3-C4-C41 & 110.89 (13) & C45-C44-H44 & 120.00 \\ O3-C4-C5 & 108.53 (12) & C44-C45-H45 & 120.00 \\ O3-C4-C41 & 113.20 (12) & C41-C46-H46 & 119.00 \\ C4-C5-C15 & 115.43 (13) & C45-C44-H46 & 119.00 \\ C4-C5-C15 & 115.43 (13) & C45-C44-H46 & 119.00 \\ C4-C5-C15 & 115.43 (13) & C6-C61-H61B & 109.00 \\ N1-C6-C5 & 117.44 (14) & C6-C61-H61B & 109.00 \\ N1-C6-C5 & 117.44 (13) & C6-C61-H61B & 109.00 \\ O15-C15-C16 & 112.07 (13) & C6-C61-H61B & 109.00 \\ N1-C6-C5 & 117.44 (13) & C6-C61-H61B & 109.00 \\ N1-C6-C5 & 118.27 (17) & H61A-C61-H61B & 19.00 \\ O15-C15-C16 & 113.09 (14) & C6-C61-H61B & 19.00 \\ O15-C15-C16 & 113.09 (14) & C6-C61-H61B & 19.00 \\ O15-C15-C16 & 113.29 (17) & H61A-C61-H61B & 19.00 \\ O15-C15-C44 & 122.34 (17) & H61A-C61-H61B & 19.00 \\ O15-C15-C44 & 122.34 (17) & H6$	C2…H16A ^v	2.8200	H61B…C16	2.7700
C2-H3 ⁱⁱ 3.064 (19) H61B···H16C 2.3200 C5···H46 2.5100 H61B···C45 ^{vii} 3.0500 C6···H46 2.7700 H61C···C16 2.9400 C16···H61D 2.8500 H61D···C15 2.8500 C16···H61D 2.8500 H61D···C16 2.3400 C16···H61D 2.3400 H61D···H16B 1.9000 C16···H61B 2.7700 H61D···H16B 1.9000 C42···H3 3.087 (17) H61E···H1 2.4400 C42···H3 3.0500 H61F···H1 2.5000 C45···H61B ^v 3.0500 H61F···H1 2.5400 C45···H61B ^v 3.0500 H61F···H1 2.5400 C2N1C6 123.53 (13) C15C16-H16B 109.00 C2N1-H1 116.1 (14) H16A-C16-H16C 109.00 C2N3-H3 119.2 (12) H16B-C16-H16C 10.00 C4N3-H43 120.00 N1-C2-N3 124.35 (14) C44-C43-H44 120.00 N1-C2-N3 115.05 (13) C43C44-H44 120.00 </td <td>C2…H1ⁱⁱ</td> <td>2.93 (2)</td> <td>H61B…H16B</td> <td>2.5900</td>	C2…H1 ⁱⁱ	2.93 (2)	H61B…H16B	2.5900
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C2···H3 ⁱⁱⁱ	3.064 (19)	H61B…H16C	2.3200
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C5…H46	2.5100	H61B…C45 ^{vii}	3.0500
$\begin{array}{ccccc} C6-H16B & 3.0800 & H61C-H16B & 2.3400 \\ C15-H61D & 2.8500 & H61D-C15 & 2.8500 \\ C16-H61C & 2.9400 & H61D-C16 & 2.3400 \\ C16-H61D & 2.3400 & H61D-H16B & 1.9000 \\ C16-H61B & 2.7700 & H61D-H16C & 2.1900 \\ C42-H3 & 3.087 (17) & H61E-H1 & 2.4400 \\ C42-H3 & 3.087 (17) & H61E-H1 & 2.5400 \\ C45-H61B^{V} & 3.0500 & H61F-H1 & 2.5400 \\ C45-H61B^{V} & 3.0500 & H61F-H1 & 2.5400 \\ C45-H16C^{V} & 3.0100 & H61F-O15^{X} & 2.7000 \\ C2-N1-C6 & 12.353 (13) & C15-C16-H16B & 109.00 \\ C2-N3-C4 & 120.87 (13) & C15-C16-H16C & 109.00 \\ C2-N3-H1 & 116.1 (14) & H16A-C16-H16B & 109.00 \\ C2-N3-H3 & 119.2 (12) & H16B-C16-H16B & 109.00 \\ C2-N3-H3 & 119.2 (12) & H16B-C16-H16C & 110.00 \\ C4-N3-H3 & 116.7 (12) & C42-C43-H43 & 120.00 \\ 02-C2-N3 & 124.35 (14) & C44-C43-H43 & 120.00 \\ 02-C2-N3 & 126.81 (13) & C45-C44-H44 & 120.00 \\ 02-C2-N1 & 120.58 (13) & C45-C44-H44 & 120.00 \\ 02-C2-N1 & 120.58 (13) & C45-C44-H44 & 120.00 \\ 02-C2-N1 & 13.20 (12) & C41-C45-H45 & 120.00 \\ 02-C2-N1 & 13.20 (12) & C41-C45-H45 & 120.00 \\ 02-C2-N1 & 13.20 (12) & C41-C46-H46 & 119.00 \\ C4-C5-C15 & 115.43 (13) & C45-C46-H46 & 119.00 \\ C4-C5-C15 & 115.43 (13) & C45-C46-H46 & 119.00 \\ C4-C5-C15 & 115.43 (13) & C45-C46-H46 & 119.00 \\ C4-C5-C5 & 115.43 (13) & C45-C46-H46 & 119.00 \\ C4-C5-C5 & 115.43 (13) & C45-C46-H46 & 119.00 \\ C4-C5-C5 & 115.43 (13) & C45-C46-H46 & 119.00 \\ C4-C5-C5 & 115.43 (13) & C45-C46-H46 & 119.00 \\ C5-C4-C41 & 13.20 (12) & C41-C46-H46 & 119.00 \\ C5-C4-C5 & 115.43 (13) & C6-C61-H61B & 109.00 \\ N1-C6-C5 & 115.43 (13) & C6-C61-H61B & 109.00 \\ N1-C6-C5 & 115.43 (13) & C6-C61-H61B & 109.00 \\ C5-C5-C15-C16 & 123.34 (17) & C6-C61-H61B & 109.00 \\ C4-C15-C15-C16 & 118.39 (17) & H61A-C61-H61B & 109.00 \\ C4-C41-C46 & 122.25 (14) & H61A-C61-H61B & 109.00 \\ C4-C41-C46 & 122.25 (14) & H61A-C61-H61B & 109.00 \\ C4-C41-C46 & 122.5 (14) & H61A-C61-H61B & 109.00 \\ C4-C41-C46 & 122.5 (14) & H61A-C61-H61B & 109.00 \\ C4-C41-C46 & 122.5 (14) & H61A-C61-H61B & 109.00 \\ C1-C42-C43 & 117.92 (15) & H61B-C61-H61D & 141.00 \\ C1-C42-C43 & 117.92 (15) & H61B-C61-H61D & $	С6…Н46	2.7700	H61C…C16	2.9400
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6…H16B	3.0800	H61C…H16B	2.3400
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C15…H61D	2.8500	H61D…C15	2.8500
$\begin{array}{cccccccc} C16 - H61B & 2.3400 & H61D - H16B & 1.9000 \\ C16 - H61B & 2.7700 & H61D - H16C & 2.1900 \\ C41 - H45^{1v} & 3.0100 & H61E - H1 & 2.4400 \\ C42 - H3 & 3.087 (17) & H61E - H4^{1x} & 2.3100 \\ C45 - H61B^{V} & 3.0500 & H61F - H1 & 2.5400 \\ C45 - H16C^{V} & 3.0100 & H61F - O15^{8} & 2.7000 \\ C2 - N1 - C6 & 123.53 (13) & C15 - C16 - H16B & 109.00 \\ C2 - N3 - C4 & 120.87 (13) & C15 - C16 - H16C & 109.00 \\ C2 - N3 - C4 & 120.87 (13) & C15 - C16 - H16C & 109.00 \\ C2 - N1 - H1 & 116.1 (14) & H16A - C16 - H16C & 109.00 \\ C2 - N3 - H3 & 119.2 (12) & H16B - C16 - H16C & 110.00 \\ C4 - N3 - H3 & 116.7 (12) & C42 - C43 - H43 & 120.00 \\ N1 - C2 - N3 & 123.53 (14) & C44 - C43 - H44 & 120.00 \\ N3 - C4 - C5 & 108.53 (12) & C44 - C44 - H44 & 120.00 \\ N3 - C4 - C5 & 108.53 (12) & C44 - C45 - H45 & 120.00 \\ N3 - C4 - C5 & 108.53 (12) & C44 - C45 - H45 & 120.00 \\ C4 - C5 - C15 & 127.40 (14) & C6 - C61 - H61B & 109.00 \\ C4 - C5 - C15 & 177.40 (14) & C6 - C61 - H61B & 109.00 \\ C4 - C5 - C15 & 177.40 (14) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ N1 - C6 - C5 & 117.84 (13) & C6 - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 123.34 (17) & C6 - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 118.27 (17) & H61A - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 118.27 (17) & H61A - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 118.27 (17) & H61A - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 118.39 (17) & H61A - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 118.27 (17) & H61A - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 118.27 (17) & H61A - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 118.27 (17) & H61A - C61 - H61B & 109.00 \\ O15 - C15 - C16 & 118$	C16…H61C	2.9400	H61D…C16	2.3400
$\begin{array}{ccccccc} C16 \cdots H61B & 2.7700 & H61D \cdots H16C & 2.1900 \\ C41 \cdots H45^{1v} & 3.0100 & H61E \cdots H1 & 2.4400 \\ C42 \cdots H3 & 3.087 (17) & H61E \cdots H4^{1x} & 2.3100 \\ C45 \cdots H61B^{V} & 3.0500 & H61F \cdots H1 & 2.5400 \\ C45 \cdots H16C^{V} & 3.0100 & H61F \cdots H1 & 2.5400 \\ C45 \cdots H16C^{V} & 3.0100 & H61F \cdots D15^{S} & 2.7000 \\ C2 = N1 = C6 & 123.53 (13) & C15 = C16 = H16B & 109.00 \\ C2 = N3 = C4 & 120.87 (13) & C15 = C16 = H16B & 109.00 \\ C2 = N3 = C4 & 120.87 (13) & C15 = C16 = H16B & 109.00 \\ C2 = N3 = H1 & 116.1 (14) & H16A = C16 = H16C & 109.00 \\ C2 = N3 = H3 & 119.2 (12) & H16B = C16 = H16C & 110.00 \\ C4 = N3 = H3 & 116.7 (12) & C42 = C43 = H43 & 120.00 \\ O2 = C2 = N3 & 124.35 (14) & C44 = C43 = H43 & 120.00 \\ O3 = C4 = C5 & 108.53 (12) & C44 = C44 = H44 & 120.00 \\ N3 = C4 = C5 & 108.53 (12) & C44 = C45 = H45 & 120.00 \\ N3 = C4 = C5 & 108.53 (12) & C44 = C45 = H45 & 120.00 \\ C4 = C5 = C15 & 127.40 (14) & C6 = C61 = H61A & 109.00 \\ C4 = C5 = C15 & 17.84 (13) & C6 = C61 = H61B & 109.00 \\ C4 = C5 = C15 & 17.12 (13) & C6 = C61 = H61B & 109.00 \\ N1 = C6 = C5 & 117.84 (13) & C6 = C61 = H61B & 109.00 \\ N1 = C6 = C5 & 117.84 (13) & C6 = C61 = H61B & 109.00 \\ N1 = C6 = C5 & 117.84 (13) & C6 = C61 = H61B & 109.00 \\ N1 = C6 = C5 & 117.84 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 112.07 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 112.07 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 112.07 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 112.07 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 112.07 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 112.07 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 112.07 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 112.07 (13) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 113.09 (14) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 113.09 (14) & C6 = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 118.39 (17) & H61A = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 118.39 (17) & H61A = C61 = H61B & 109.00 \\ O15 = C15 = C16 & 116.41 (15) & H61A = C61 = H61B & 109.00 \\ O15 = C15 = C16$	C16…H61D	2.3400	H61D…H16B	1.9000
C41···H45 ^{iv} 3.0100H61E···H12.4400C42···H33.087 (17)H61E···H12.3100C45···H61B ^v 3.0500H61F···H12.5400C45···H16C ^v 3.0100H61F···O15 ^x 2.7000C2N1-C6123.53 (13)C15C16H16B109.00C2N3-C4120.87 (13)C15C16H16C109.00C2N1-H1116.1 (14)H16AC16H16C109.00C2N3-H3119.2 (12)H16BC16H16C109.00C2N3-H3116.7 (12)C42C43H43120.00O2C2-N3124.35 (14)C44C43H43120.00O2C2-N3115.05 (13)C43C44H44120.00N1C2-N3115.05 (13)C45C44H44120.00N3C4-C5108.53 (12)C44C45H45120.00N3C4-C41113.20 (12)C41C46H46119.00C4C5-C15115.43 (13)C45C44H46119.00C4C5-C15115.43 (13)C45C46H46119.00C4C5-C15117.84 (13)C6C61H61A109.00N1C6-C61112.07 (13)C6C61H61B109.00N1C6-C61112.07 (13)C6C61H61B109.00N1C6-C61112.07 (13)C6C61H61B109.00O15C15-C16123.34 (17)C6C61H61B109.00O15C15-C16123.34 (17)C6C61H61B109.00O15C15-C16118.39 (17)H61AC61H61B109.00O15C15-C16118.39 (17)H61AC61H61D141.00C4	C16…H61B	2.7700	H61D…H16C	2.1900
C42-··H3 $3.087 (17)$ $H61E-··H4^{ix}$ 2.3100 C45···H61B ^v 3.0500 H61F···H1 2.5400 C45···H16C ^v 3.0100 H61F···O15 ^x 2.7000 C2N1C6123.53 (13)C15C16H16B109.00C2N3C4120.87 (13)C15C16H16C109.00C2N1H1116.1 (14)H16AC16H16C109.00C4N3H3119.2 (12)H16BC16H16C109.00C2N3H3116.7 (12)C42C43H43120.00C2C2N3124.35 (14)C44C43H43120.00C2C2N3115.05 (13)C43C44H44120.00C2C2N1120.58 (13)C45C44H44120.00C3C4C5108.53 (12)C44C45H45120.00N3C4C5108.53 (12)C44C45H45120.00C4C5C15115.43 (13)C45C46H46119.00C4C5-C15127.40 (14)C6C61H61A109.00C4C5-C1517.84 (13)C6C61H61B109.00C5C15-C16123.34 (17)C6C61H61D109.00C5C15-C16123.34 (17)C6C61H61B109.00C5C15-C16123.34 (17)C6C61H61B109.00C5C15-C16123.34 (17)C6C61H61B109.00C5C15-C16123.34 (17)C6C61H61B109.00C5C15-C16123.34 (17)C6C61H61D141.00C4C41C46118.39 (17)H61AC61H61D141.00C4C41C46118.39 (17)H61AC61H61D<	C41···H45 ^{iv}	3.0100	H61E…H1	2.4400
C45H61B ^v 3.0500H61FH12.5400C45H16C ^v 3.0100H61FO15 ^x 2.7000C2N1C6123.53 (13)C15C16H16B109.00C2N3C4120.87 (13)C15C16H16C109.00C2N1H1116.1 (14)H16AC16H16C109.00C6N1H1119.4 (14)H16AC16H16C110.00C4N3H3119.2 (12)H16BC16H16C110.00C4N3H3116.7 (12)C42C43H43120.00O2C2N3124.35 (14)C44C43H43120.00O2C2N3115.05 (13)C43C44H44120.00N3C4C5108.53 (12)C44C45H45120.00N3C4C5108.53 (12)C44C45H45120.00C5C4C41113.20 (12)C41C46H46119.00C4C5-C15115.43 (13)C45C46H46119.00C4C5-C6117.12 (13)C6C61H61B109.00N1C6-C5117.84 (13)C6C61H61B109.00N1C6-C5117.84 (13)C6C61H61B109.00N1C6-C5118.27 (17)H61AC61H61B109.00O5C5-C16123.34 (17)C6C61H61B109.00O5C15-C16118.39 (17)H61AC61H61B109.00O15C15-C16118.39 (17)H61AC61H61B109.00O15C15C16118.39 (17)H61AC61H61B109.00O15C15C16118.39 (17)H61AC61H61B109.00O15C15C16118.39 (17)H61AC61H61B	С42…Н3	3.087 (17)	H61E…H4 ^{ix}	2.3100
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C45…H61B ^v	3.0500	H61F…H1	2.5400
$\begin{array}{ccccccc} C12-N1-C6&123.53(13)&C15-C16-H16B&109.00\\ C2-N3-C4&120.87(13)&C15-C16-H16C&109.00\\ C2-N1-H1&116.1(14)&H16A-C16-H16C&109.00\\ C6-N1-H1&119.4(14)&H16A-C16-H16C&109.00\\ C2-N3-H3&119.2(12)&H16B-C16-H16C&110.00\\ C4-N3-H3&116.7(12)&C42-C43-H43&120.00\\ O2-C2-N3&124.35(14)&C44-C43-H43&120.00\\ O2-C2-N3&115.05(13)&C43-C44-H44&120.00\\ O2-C2-N1&120.58(13)&C45-C44-H44&120.00\\ O3-C4-C5&108.53(12)&C44-C45-H45&120.00\\ N3-C4-C5&108.53(12)&C44-C45-H45&120.00\\ C5-C4-C41&110.89(13)&C45-C46-H46&119.00\\ C4-C5-C15&115.43(13)&C45-C46-H46&119.00\\ C4-C5-C15&115.43(13)&C45-C46-H46&119.00\\ C4-C5-C6&117.12(13)&C6-C61-H61B&109.00\\ C4-C5-C6&117.12(13)&C6-C61-H61B&109.00\\ C5-C6-C61&120.09(14)&C6-C61-H61B&109.00\\ C5-C6-C61&120.09(14)&C6-C61-H61B&109.00\\ C5-C6-C61&130.09(14)&C6-C61-H61B&109.00\\ C5-C6-C61&130.09(14)&C6-C61-H61B&109.00\\ C4-C5-C5&117.84(13)&C6-C61-H61B&109.00\\ C5-C6-C61&130.09(14)&C6-C61-H61B&109.00\\ C4-C5-C5&118.27(17)&H61A-C61-H61B&109.00\\ C4-C41-C46&122.25(14)&H61A-C61-H61B&109.00\\ C4-C41-C46&122.25(14)&H61A-C61-H61B&109.00\\ C4-C41-C46&122.25(14)&H61A-C61-H61B&109.00\\ C4-C41-C46&122.25(14)&H61A-C61-H61B&109.00\\ C4-C41-C46&122.25(14)&H61A-C61-H61B&109.00\\ C4-C41-C46&122.25(14)&H61A-C61-H61D&141.00\\ C4-C41-C42&121.34(13)&H61A-C61-H61D&140\\ C10-C61-H61D&141.00\\ C4-C41-C42&121.34(13)&H61A-C61-H61D&140\\ C10-C61-H61D&140\\ C10-C61-H61D&140\\ C10-C61-H61D&140\\ C10-C61-H61D&140\\ C10-C61-H61D&140\\ C10-C61-H61D&140\\ C10-C61-H61D&140\\ C10-C61-H61D&140\\ C10-C61-H61D&14$	C45…H16C ^v	3.0100	H61F…O15 ^x	2.7000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—N1—C6	123.53 (13)	C15—C16—H16B	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—N3—C4	120.87 (13)	C15—C16—H16C	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—N1—H1	116.1 (14)	H16A—C16—H16B	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6—N1—H1	119.4 (14)	H16A—C16—H16C	109.00
C4-N3-H3116.7 (12)C42-C43-H43120.00O2-C2-N3124.35 (14)C44-C43-H43120.00N1-C2-N3115.05 (13)C43-C44-H44120.00O2-C2-N1120.58 (13)C45-C44-H44120.00N3-C4-C5108.53 (12)C44-C45-H45120.00N3-C4-C41110.89 (13)C46-C45-H45120.00C5-C4-C41113.20 (12)C41-C46-H46119.00C4-C5-C15115.43 (13)C45-C46-H46119.00C4-C5-C15127.40 (14)C6-C61-H61A109.00C4-C5-C6117.12 (13)C6-C61-H61B109.00N1-C6-C5117.84 (13)C6-C61-H61D109.00N1-C6-C61112.07 (13)C6-C61-H61E109.00C5-C15-C16123.34 (17)C6-C61-H61E109.00C5-C15-C5118.27 (17)H61A-C61-H61B109.00O15-C15-C5118.27 (17)H61A-C61-H61D141.00C4-C41-C46122.25 (14)H61A-C61-H61D141.00C4-C41-C46122.25 (14)H61A-C61-H61E56.00C4-C41-C42121.34 (13)H61A-C61-H61E56.00C11-C42-C41119.65 (13)H61B-C61-H61D109.00C11-C42-C43117.92 (15)H61B-C61-H61D56.00	C2—N3—H3	119.2 (12)	H16B—C16—H16C	110.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4—N3—H3	116.7 (12)	C42—C43—H43	120.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—C2—N3	124.35 (14)	C44—C43—H43	120.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1—C2—N3	115.05 (13)	C43—C44—H44	120.00
N3-C4-C5108.53 (12)C44-C45-H45120.00N3-C4-C41110.89 (13)C46-C45-H45120.00C5-C4-C41113.20 (12)C41-C46-H46119.00C4-C5-C15115.43 (13)C45-C46-H46119.00C6-C5-C15127.40 (14)C6-C61-H61A109.00C4-C5-C6117.12 (13)C6-C61-H61B109.00N1-C6-C5117.84 (13)C6-C61-H61D109.00N1-C6-C61112.07 (13)C6-C61-H61D109.00C5-C4-C61130.09 (14)C6-C61-H61E109.00C5-C15-C16123.34 (17)C6-C61-H61B109.00O15-C15-C5118.27 (17)H61A-C61-H61B109.00O15-C15-C16118.39 (17)H61A-C61-H61D141.00C4-C41-C46122.25 (14)H61A-C61-H61D141.00C4-C41-C46116.41 (15)H61A-C61-H61E56.00C11-C42-C41119.65 (13)H61B-C61-H61D109.00C11-C42-C43117.92 (15)H61B-C61-H61D56.00	O2—C2—N1	120.58 (13)	C45—C44—H44	120.00
N3C4C41110.89 (13)C46C45H45120.00C5C4C41113.20 (12)C41C46H46119.00C4C5C15115.43 (13)C45C46H46119.00C6C5C15127.40 (14)C6C61H61A109.00C4C5C6117.12 (13)C6C61H61B109.00N1C6C5117.84 (13)C6C61H61D109.00N1C6C61112.07 (13)C6C61H61D109.00C5C15C16123.34 (17)C6C61H61E109.00C5C15C16123.34 (17)C6C61H61B109.00O15C15C16118.27 (17)H61AC61H61B109.00O15C15C16118.39 (17)H61AC61H61D141.00C4C41C46122.25 (14)H61AC61H61D141.00C4C41C42121.34 (13)H61AC61H61F56.00C11C42C41119.65 (13)H61BC61H61D109.00C11C42C43117.92 (15)H61BC61H61D56.00	N3—C4—C5	108.53 (12)	C44—C45—H45	120.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N3—C4—C41	110.89 (13)	C46—C45—H45	120.00
C4—C5—C15115.43 (13)C45—C46—H46119.00C6—C5—C15127.40 (14)C6—C61—H61A109.00C4—C5—C6117.12 (13)C6—C61—H61B109.00N1—C6—C5117.84 (13)C6—C61—H61D109.00N1—C6—C61112.07 (13)C6—C61—H61D109.00C5—C6—C61130.09 (14)C6—C61—H61E109.00C5—C15—C16123.34 (17)C6—C61—H61F109.00O15—C15—C5118.27 (17)H61A—C61—H61B109.00O15—C15—C16122.25 (14)H61A—C61—H61D141.00C4—C41—C46122.25 (14)H61A—C61—H61D141.00C4—C41—C46116.41 (15)H61A—C61—H61F56.00C4—C41—C42121.34 (13)H61A—C61—H61F56.00C11—C42—C41119.65 (13)H61B—C61—H61D109.00C11—C42—C43117.92 (15)H61B—C61—H61D56.00	C5—C4—C41	113.20 (12)	C41—C46—H46	119.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4—C5—C15	115.43 (13)	C45—C46—H46	119.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6—C5—C15	127.40 (14)	С6—С61—Н61А	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4—C5—C6	117.12 (13)	С6—С61—Н61В	109.00
N1—C6—C61 $112.07 (13)$ C6—C61—H61D 109.00 C5—C6—C61 $130.09 (14)$ C6—C61—H61E 109.00 C5—C15—C16 $123.34 (17)$ C6—C61—H61F 109.00 O15—C15—C5 $118.27 (17)$ H61A—C61—H61B 109.00 O15—C15—C16 $118.39 (17)$ H61A—C61—H61C 109.00 C4—C41—C46 $122.25 (14)$ H61A—C61—H61D 141.00 C4—C41—C46 $116.41 (15)$ H61A—C61—H61E 56.00 C4—C41—C42 $121.34 (13)$ H61A—C61—H61F 56.00 C11—C42—C41 $119.65 (13)$ H61B—C61—H61C 109.00 C11—C42—C43 $117.92 (15)$ H61B—C61—H61D 56.00	N1—C6—C5	117.84 (13)	С6—С61—Н61С	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1—C6—C61	112.07 (13)	C6—C61—H61D	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5—C6—C61	130.09 (14)	С6—С61—Н61Е	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5—C15—C16	123.34 (17)	C6—C61—H61F	109.00
O15—C15—C16118.39 (17)H61A—C61—H61C109.00C4—C41—C46122.25 (14)H61A—C61—H61D141.00C42—C41—C46116.41 (15)H61A—C61—H61E56.00C4—C41—C42121.34 (13)H61A—C61—H61F56.00C11—C42—C41119.65 (13)H61B—C61—H61C109.00C11—C42—C43117.92 (15)H61B—C61—H61D56.00	O15—C15—C5	118.27 (17)	H61A—C61—H61B	109.00
C4—C41—C46122.25 (14)H61A—C61—H61D141.00C42—C41—C46116.41 (15)H61A—C61—H61E56.00C4—C41—C42121.34 (13)H61A—C61—H61F56.00C11—C42—C41119.65 (13)H61B—C61—H61C109.00C11—C42—C43117.92 (15)H61B—C61—H61D56.00	O15—C15—C16	118.39 (17)	H61A—C61—H61C	109.00
C42—C41—C46 116.41 (15) H61A—C61—H61E 56.00 C4—C41—C42 121.34 (13) H61A—C61—H61F 56.00 C11—C42—C41 119.65 (13) H61B—C61—H61C 109.00 C11—C42—C43 117.92 (15) H61B—C61—H61D 56.00	C4—C41—C46	122.25 (14)	H61A—C61—H61D	141.00
C4—C41—C42121.34 (13)H61A—C61—H61F56.00C11—C42—C41119.65 (13)H61B—C61—H61C109.00C11—C42—C43117.92 (15)H61B—C61—H61D56.00	C42—C41—C46	116.41 (15)	H61A—C61—H61E	56.00
Cl1—C42—C41119.65 (13)H61B—C61—H61C109.00Cl1—C42—C43117.92 (15)H61B—C61—H61D56.00	C4—C41—C42	121.34 (13)	H61A—C61—H61F	56.00
Cl1—C42—C43 117.92 (15) H61B—C61—H61D 56.00	Cl1—C42—C41	119.65 (13)	H61B—C61—H61C	109.00
	Cl1—C42—C43	117.92 (15)	H61B—C61—H61D	56.00

C41—C42—C43	122.43 (18)	H61B—C61—H61E	141.00
C42—C43—C44	119.20 (19)	H61B—C61—H61F	56.00
C43—C44—C45	120.20 (19)	H61C—C61—H61D	56.00
C44—C45—C46	119.66 (18)	H61C—C61—H61E	56.00
C41—C46—C45	122.08 (16)	H61C—C61—H61F	141.00
N3—C4—H4	108.00	H61D—C61—H61E	109.00
С5—С4—Н4	108.00	H61D—C61—H61F	109.00
C41—C4—H4	108.00	H61E—C61—H61F	109.00
C15—C16—H16A	109.00		
C6—N1—C2—O2	-161.31 (14)	C15—C5—C6—N1	177.02 (15)
C6—N1—C2—N3	16.9 (2)	C15—C5—C6—C61	-3.7 (3)
C2—N1—C6—C5	-23.4 (2)	C4—C5—C15—O15	-3.9 (2)
C2—N1—C6—C61	157.25 (15)	C4—C5—C15—C16	175.71 (16)
C4—N3—C2—O2	-162.51 (15)	C6-C5-C15-O15	173.16 (17)
C4—N3—C2—N1	19.4 (2)	C6-C5-C15-C16	-7.3 (3)
C2—N3—C4—C5	-44.08 (19)	C4—C41—C42—Cl1	2.9 (2)
C2—N3—C4—C41	80.86 (17)	C4—C41—C42—C43	-177.59 (16)
N3—C4—C5—C6	35.79 (18)	C46—C41—C42—Cl1	-177.91 (12)
N3—C4—C5—C15	-146.88 (14)	C46—C41—C42—C43	1.6 (2)
C41—C4—C5—C6	-87.77 (16)	C4—C41—C46—C45	177.56 (15)
C41—C4—C5—C15	89.56 (16)	C42—C41—C46—C45	-1.6 (2)
N3—C4—C41—C42	66.67 (18)	Cl1—C42—C43—C44	179.21 (15)
N3-C4-C41-C46	-112.46 (16)	C41—C42—C43—C44	-0.3 (3)
C5—C4—C41—C42	-171.08 (14)	C42—C43—C44—C45	-1.1 (3)
C5—C4—C41—C46	9.8 (2)	C43—C44—C45—C46	1.0 (3)
C4-C5-C6-N1	-6.0 (2)	C44—C45—C46—C41	0.4 (3)
C4—C5—C6—C61	173.24 (15)		

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) -*x*+1, -*y*+1, *z*+1/2; (iii) -*x*+1, -*y*+1, *z*-1/2; (iv) -*x*+1, -*y*, *z*+1/2; (v) *x*+1/2, -*y*+1/2, *z*; (vi) -*x*+1/2, *y*-1/2, *z*+1/2; (vii) *x*-1/2, -*y*+1/2, *z*; (vii) -*x*+1, -*y*, *z*-1/2; (ix) *x*, *y*, *z*-1; (x) -*x*+1/2, *y*+1/2, *z*-1/2.

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A
N1—H1···O2 ⁱⁱⁱ	0.80 (2)	2.05 (2)	2.8386 (18)	170.6 (19)
N3—H3…Cl1	0.83 (2)	2.748 (18)	3.2005 (15)	116.2 (14)
N3—H3···O2 ⁱⁱ	0.83 (2)	2.18 (2)	2.9627 (18)	158.6 (16)
C4—H4…O15	0.98	2.35	2.712 (2)	101
C16—H16A····O2 ^{vii}	0.96	2.51	3.421 (2)	159
C45—H45···O15 ^{viii}	0.93	2.55	3.257 (3)	133
C16—H16C···Cg ^{vii}	0.96	2.86	3.699 (2)	147

Symmetry codes: (iii) -x+1, -y+1, z-1/2; (ii) -x+1, -y+1, z+1/2; (vii) x-1/2, -y+1/2, z; (viii) -x+1, -y, z-1/2.





