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Ethyl 2-allyl-2-(5-methyl-1,2,4-triazolo[1,5-*a*]-pyrimidin-7-yl)pent-4-enoate

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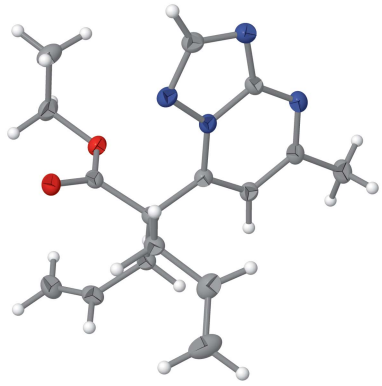
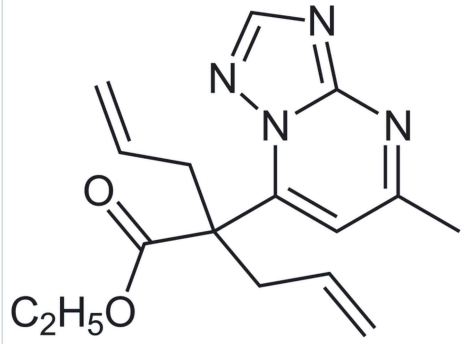
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{16}H_{20}N_4O_2$, the dihedral angle between the planes of the fused rings is 2.26 (8)°. In the crystal, [$\bar{2}$10] chains of molecules linked by C—H···O and C—H···N hydrogen bonds arise, which are further linked by weak C—H···π interactions.

3D view



Chemical scheme



Structure description

Triazolopyrimidine derivatives display various pharmacological properties, including anti-inflammatory (Ashour *et al.*, 2013), anticancer (Hoffmann *et al.*, 2017) and anti-bacterial (Mabkhot *et al.*, 2016) activities. The present work is a continuation of our structural studies of triazolopyrimidine derivatives (Lahmidi *et al.*, 2016) and reports the synthesis and structure of the title compound, ethyl 2-allyl-2-(5-methyl-1,2,4-triazolo-[1,5-*a*]pyrimidin-7-yl)pent-4-enoate (Fig. 1).

The bicyclic unit is slightly nonplanar, as indicated by the dihedral angle of 2.26 (8)° between the planes of the five- and six-membered rings. In the crystal, molecules form centrosymmetric dimers through complementary C1—H1···O1^{i} hydrogen bonds, which are connected into [$\bar{2}$10] chains by C16—H16*A*···N4^{ii} hydrogen bonds (Table 1 and Fig. 2). The chains are connected by C12—H12···*Cg*1^{iii} (*Cg*1 is the centroid of the C1/N3/C2/N1/N2 ring) interactions (Table 1 and Figs. 2 and 3).

Synthesis and crystallization

Allyl bromide (0.22 ml, 2.5 mmol), potassium carbonate (0.34 g, 2.5 mmol) and a catalytic quantity of tetra-*n*-butylammonium iodide were added to a solution of ethyl 2-(5-methyl-

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{i}	0.962 (14)	2.315 (14)	3.2388 (15)	160.7 (11)
C16—H16A···N4^{ii}	0.976 (16)	2.610 (16)	3.4354 (18)	142.4 (12)
C12—H12···Cg1^{iii}	0.981 (15)	2.955 (15)	3.6559 (15)	129.3 (11)

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

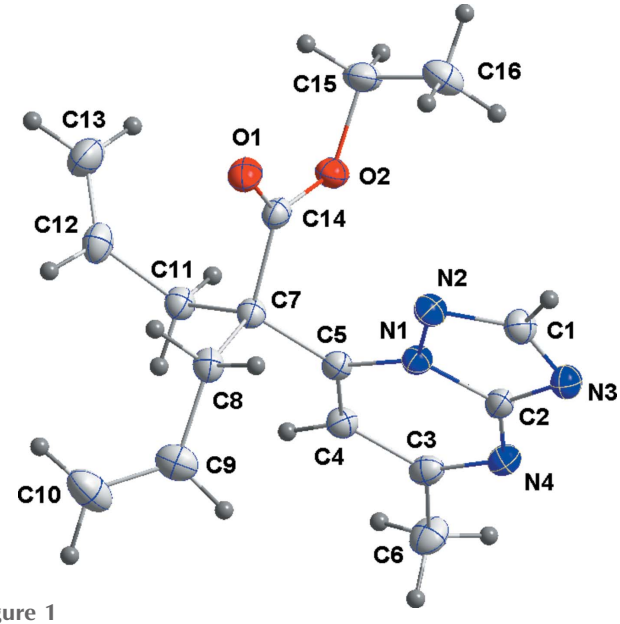


Figure 1
The title molecule, shown with 50% probability displacement ellipsoids.

1,2,4-triazolo[1,5-*a*]pyrimidin-7-yl)acetate (0.5 g, 2.3 mmol) in DMF (15 ml). The mixture was stirred at room temperature for 48 h. The solution was filtered and the solvent removed under reduced pressure. The resulting residue was purified by column chromatography (EtOAc–hexane 1/9 *v*/*v*). The title compound was recrystallized from an ethanol solution at room temperature to yield colourless plates (yield 30%; m.p. 364–366 K).

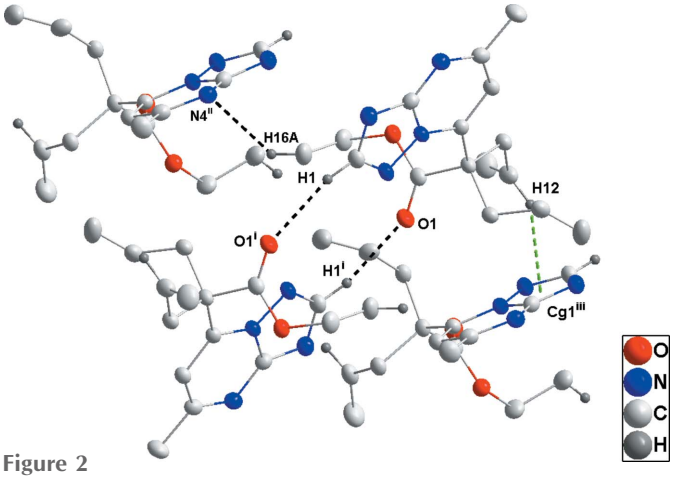


Figure 2
Detail of the intermolecular interactions, with C—H···O and C—H···N hydrogen bonds shown as black dashed lines, while the C—H···π(ring) is shown as a green dashed line. [Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.]

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{20}N_4O_2$
M_r	300.36
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	10.0937 (9), 13.4926 (12), 11.6936 (11)
β (°)	92.999 (1)
V (Å^3)	1590.4 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.30 × 0.24 × 0.07
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.83, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14774, 3914, 2819
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.111, 1.03
No. of reflections	3914
No. of parameters	279
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.18

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal and refinement data are presented in Table 2. The H atoms were located in difference maps and their positions and U_{iso}(H) values were refined freely.

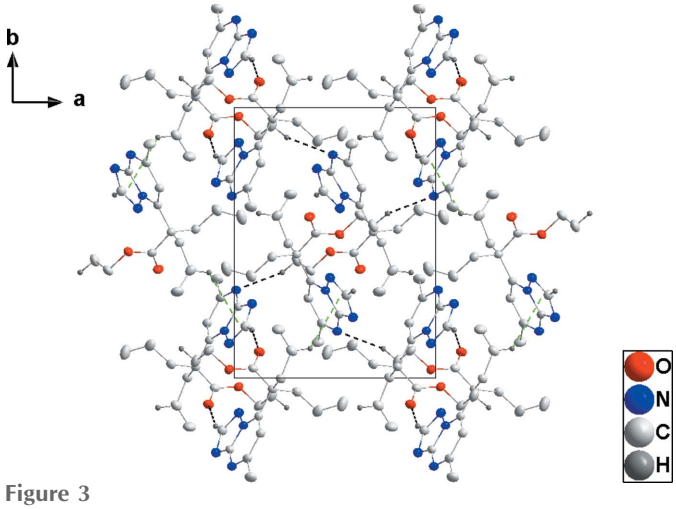


Figure 3
The packing of the title compound, viewed along the *c*-axis direction, with intermolecular interactions depicted as in Fig. 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171243 [https://doi.org/10.1107/S2414314617012433]

Ethyl 2-allyl-2-(5-methyl-1,2,4-triazolo[1,5-*a*]pyrimidin-7-yl)pent-4-enoate

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Crystal data

$C_{16}H_{20}N_4O_2$
M_r = 300.36
Monoclinic, $P2_1/n$
a = 10.0937 (9) Å
b = 13.4926 (12) Å
c = 11.6936 (11) Å
β = 92.999 (1)°
V = 1590.4 (2) Å^3
Z = 4
$F(000)$ = 640
D_x = 1.254 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4361 reflections
θ = 2.3–27.5°
μ = 0.09 mm^{-1}
T = 100 K
Plate, colourless
0.30 × 0.24 × 0.07 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.83, T_{max} = 0.99
14774 measured reflections
3914 independent reflections
2819 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 28.3°, θ_{min} = 2.3°
h = −13→13
k = −17→17
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.111
S = 1.03
3914 reflections
279 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

Experimental. The diffraction data were collected in three sets of 363 frames (0.5° width in ω) at φ = 0, 120 and 240°. A scan time of 40 sec/frame was used.

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.37418 (8)	0.59703 (6)	0.81629 (7)	0.0269 (2)
O2	0.52312 (8)	0.53189 (6)	0.70030 (7)	0.0237 (2)
N1	0.45281 (9)	0.32484 (7)	0.77637 (8)	0.0195 (2)
N2	0.47572 (10)	0.37149 (8)	0.87926 (8)	0.0231 (2)
N3	0.58922 (10)	0.22459 (8)	0.87571 (9)	0.0252 (3)
N4	0.51065 (10)	0.17365 (7)	0.68593 (9)	0.0230 (2)
C1	0.55721 (12)	0.30760 (9)	0.93342 (11)	0.0245 (3)
H1	0.5901 (13)	0.3219 (10)	1.0103 (12)	0.027 (4)*
C2	0.52088 (11)	0.23590 (9)	0.77578 (10)	0.0207 (3)
C3	0.43401 (12)	0.20285 (9)	0.59705 (11)	0.0226 (3)
C4	0.36816 (12)	0.29598 (9)	0.59266 (10)	0.0210 (3)
H4	0.3144 (12)	0.3147 (9)	0.5254 (11)	0.019 (3)*
C5	0.37784 (11)	0.35921 (8)	0.68375 (10)	0.0189 (3)
C6	0.41670 (16)	0.13343 (11)	0.49806 (12)	0.0309 (3)
H6A	0.343 (2)	0.0885 (15)	0.5148 (17)	0.068 (6)*
H6B	0.4950 (19)	0.0955 (13)	0.4883 (15)	0.057 (5)*
H6C	0.3894 (18)	0.1684 (13)	0.4266 (16)	0.057 (5)*
C7	0.31002 (11)	0.45886 (8)	0.69306 (10)	0.0198 (3)
C8	0.18878 (12)	0.44847 (9)	0.76874 (11)	0.0222 (3)
H8A	0.2226 (13)	0.4273 (10)	0.8461 (12)	0.023 (3)*
H8B	0.1481 (13)	0.5139 (10)	0.7775 (11)	0.026 (3)*
C9	0.08519 (13)	0.37797 (11)	0.72205 (11)	0.0292 (3)
H9	0.1090 (14)	0.3062 (11)	0.7130 (12)	0.036 (4)*
C10	−0.03729 (15)	0.40450 (14)	0.69308 (13)	0.0409 (4)
H10A	−0.1047 (16)	0.3565 (12)	0.6617 (14)	0.047 (5)*
H10B	−0.0668 (18)	0.4742 (14)	0.7006 (15)	0.058 (5)*
C11	0.26878 (13)	0.49788 (9)	0.57071 (10)	0.0219 (3)
H11A	0.2026 (14)	0.4522 (11)	0.5368 (12)	0.032 (4)*
H11B	0.3478 (13)	0.4967 (10)	0.5237 (12)	0.027 (4)*
C12	0.21439 (14)	0.60122 (10)	0.57129 (11)	0.0274 (3)
H12	0.1231 (15)	0.6095 (11)	0.5947 (12)	0.036 (4)*
C13	0.27982 (17)	0.67987 (11)	0.54030 (14)	0.0383 (4)
H13A	0.373 (2)	0.6753 (14)	0.5132 (16)	0.065 (6)*

H13B	0.2415 (16)	0.7449 (13)	0.5415 (14)	0.051 (5)*
C14	0.40517 (12)	0.53624 (8)	0.74715 (10)	0.0213 (3)
C15	0.62385 (14)	0.60166 (10)	0.74566 (13)	0.0290 (3)
H15A	0.5776 (15)	0.6664 (11)	0.7541 (12)	0.035 (4)*
H15B	0.6865 (14)	0.6049 (11)	0.6882 (13)	0.032 (4)*
C16	0.68866 (14)	0.56365 (12)	0.85544 (13)	0.0329 (3)
H16A	0.7608 (15)	0.6089 (11)	0.8776 (13)	0.038 (4)*
H16B	0.7315 (16)	0.4978 (13)	0.8408 (13)	0.041 (4)*
H16C	0.6263 (15)	0.5586 (11)	0.9181 (13)	0.039 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0307 (5)	0.0223 (5)	0.0272 (5)	0.0025 (4)	−0.0037 (4)	−0.0072 (4)
O2	0.0236 (4)	0.0226 (5)	0.0246 (5)	−0.0033 (3)	−0.0010 (4)	−0.0015 (3)
N1	0.0227 (5)	0.0183 (5)	0.0173 (5)	−0.0003 (4)	−0.0009 (4)	−0.0019 (4)
N2	0.0262 (5)	0.0244 (5)	0.0183 (5)	−0.0010 (4)	−0.0035 (4)	−0.0021 (4)
N3	0.0257 (6)	0.0244 (6)	0.0251 (6)	0.0010 (4)	−0.0025 (4)	0.0015 (4)
N4	0.0257 (5)	0.0197 (5)	0.0238 (6)	0.0005 (4)	0.0026 (4)	−0.0009 (4)
C1	0.0258 (6)	0.0266 (7)	0.0206 (7)	−0.0005 (5)	−0.0027 (5)	0.0013 (5)
C2	0.0198 (6)	0.0183 (6)	0.0240 (6)	0.0010 (5)	0.0018 (5)	0.0014 (5)
C3	0.0243 (6)	0.0204 (6)	0.0234 (6)	−0.0017 (5)	0.0048 (5)	−0.0018 (5)
C4	0.0235 (6)	0.0211 (6)	0.0183 (6)	−0.0009 (5)	0.0000 (5)	−0.0004 (5)
C5	0.0192 (6)	0.0200 (6)	0.0176 (6)	−0.0008 (4)	0.0013 (5)	0.0006 (5)
C6	0.0408 (8)	0.0251 (7)	0.0267 (7)	0.0039 (6)	0.0008 (6)	−0.0070 (6)
C7	0.0218 (6)	0.0189 (6)	0.0185 (6)	0.0015 (5)	−0.0021 (5)	−0.0022 (5)
C8	0.0238 (6)	0.0236 (7)	0.0190 (6)	0.0032 (5)	−0.0003 (5)	−0.0019 (5)
C9	0.0294 (7)	0.0353 (8)	0.0234 (7)	−0.0056 (6)	0.0054 (5)	−0.0044 (6)
C10	0.0302 (8)	0.0600 (11)	0.0319 (8)	−0.0114 (7)	−0.0046 (6)	0.0064 (7)
C11	0.0244 (6)	0.0226 (6)	0.0184 (6)	0.0017 (5)	−0.0020 (5)	−0.0011 (5)
C12	0.0316 (7)	0.0284 (7)	0.0217 (7)	0.0073 (6)	−0.0027 (5)	0.0004 (5)
C13	0.0447 (9)	0.0251 (8)	0.0441 (9)	0.0024 (7)	−0.0063 (7)	0.0061 (6)
C14	0.0252 (6)	0.0180 (6)	0.0204 (6)	0.0022 (5)	−0.0032 (5)	0.0010 (5)
C15	0.0272 (7)	0.0262 (7)	0.0332 (8)	−0.0088 (6)	−0.0008 (6)	0.0000 (6)
C16	0.0257 (7)	0.0413 (9)	0.0312 (8)	−0.0088 (6)	−0.0025 (6)	−0.0015 (6)

Geometric parameters (Å, º)

O1—C14	1.2044 (14)	C7—C11	1.5605 (16)
O2—C14	1.3377 (15)	C8—C9	1.4954 (18)
O2—C15	1.4645 (15)	C8—H8A	0.992 (14)
N1—N2	1.3668 (14)	C8—H8B	0.981 (14)
N1—C5	1.3693 (15)	C9—C10	1.314 (2)
N1—C2	1.3830 (15)	C9—H9	1.004 (15)
N2—C1	1.3290 (16)	C10—H10A	0.995 (17)
N3—C2	1.3342 (15)	C10—H10B	0.992 (18)
N3—C1	1.3553 (16)	C11—C12	1.4987 (18)
N4—C3	1.3228 (16)	C11—H11A	0.977 (14)

N4—C2	1.3449 (16)	C11—H11B	0.992 (15)
C1—H1	0.962 (14)	C12—C13	1.311 (2)
C3—C4	1.4211 (17)	C12—H12	0.981 (15)
C3—C6	1.4922 (18)	C13—H13A	1.01 (2)
C4—C5	1.3642 (16)	C13—H13B	0.960 (17)
C4—H4	0.965 (13)	C15—C16	1.500 (2)
C5—C7	1.5154 (16)	C15—H15A	0.998 (15)
C6—H6A	0.99 (2)	C15—H15B	0.947 (15)
C6—H6B	0.954 (19)	C16—H16A	0.976 (16)
C6—H6C	0.986 (18)	C16—H16B	1.007 (17)
C7—C14	1.5326 (16)	C16—H16C	0.993 (16)
C7—C8	1.5536 (17)		

C14—O2—C15	116.06 (10)	C9—C8—H8B	108.8 (8)
N2—N1—C5	126.97 (10)	C7—C8—H8B	109.0 (8)
N2—N1—C2	110.05 (9)	H8A—C8—H8B	106.8 (11)
C5—N1—C2	122.96 (10)	C10—C9—C8	123.45 (15)
C1—N2—N1	101.11 (10)	C10—C9—H9	117.5 (8)
C2—N3—C1	102.46 (10)	C8—C9—H9	119.0 (8)
C3—N4—C2	116.47 (10)	C9—C10—H10A	122.2 (9)
N2—C1—N3	117.16 (11)	C9—C10—H10B	121.2 (10)
N2—C1—H1	119.4 (8)	H10A—C10—H10B	116.6 (14)
N3—C1—H1	123.5 (8)	C12—C11—C7	112.95 (10)
N3—C2—N4	128.89 (11)	C12—C11—H11A	110.2 (8)
N3—C2—N1	109.21 (10)	C7—C11—H11A	107.6 (8)
N4—C2—N1	121.86 (11)	C12—C11—H11B	108.8 (8)
N4—C3—C4	123.02 (11)	C7—C11—H11B	108.6 (8)
N4—C3—C6	117.55 (11)	H11A—C11—H11B	108.6 (11)
C4—C3—C6	119.43 (11)	C13—C12—C11	124.19 (14)
C5—C4—C3	120.69 (11)	C13—C12—H12	118.6 (9)
C5—C4—H4	119.1 (7)	C11—C12—H12	117.1 (9)
C3—C4—H4	120.2 (8)	C12—C13—H13A	121.9 (11)
C4—C5—N1	114.82 (10)	C12—C13—H13B	121.8 (10)
C4—C5—C7	126.65 (11)	H13A—C13—H13B	116.3 (14)
N1—C5—C7	118.47 (10)	O1—C14—O2	124.94 (11)
C3—C6—H6A	106.9 (11)	O1—C14—C7	124.18 (11)
C3—C6—H6B	111.5 (11)	O2—C14—C7	110.67 (10)
H6A—C6—H6B	109.3 (15)	O2—C15—C16	110.70 (11)
C3—C6—H6C	111.9 (10)	O2—C15—H15A	106.2 (8)
H6A—C6—H6C	106.4 (15)	C16—C15—H15A	113.6 (8)
H6B—C6—H6C	110.7 (14)	O2—C15—H15B	104.4 (9)
C5—C7—C14	111.00 (9)	C16—C15—H15B	110.2 (9)
C5—C7—C8	109.46 (10)	H15A—C15—H15B	111.3 (12)
C14—C7—C8	108.77 (9)	C15—C16—H16A	107.4 (9)
C5—C7—C11	109.47 (9)	C15—C16—H16B	109.2 (9)
C14—C7—C11	106.26 (10)	H16A—C16—H16B	106.1 (13)
C8—C7—C11	111.86 (9)	C15—C16—H16C	112.9 (9)
C9—C8—C7	113.95 (10)	H16A—C16—H16C	109.9 (12)

C9—C8—H8A	110.5 (8)	H16B—C16—H16C	111.1 (13)
C7—C8—H8A	107.6 (8)		
C5—N1—N2—C1	−177.62 (11)	N1—C5—C7—C14	45.52 (14)
C2—N1—N2—C1	0.51 (12)	C4—C5—C7—C8	102.45 (13)
N1—N2—C1—N3	0.09 (14)	N1—C5—C7—C8	−74.56 (13)
C2—N3—C1—N2	−0.64 (14)	C4—C5—C7—C11	−20.49 (16)
C1—N3—C2—N4	−177.09 (12)	N1—C5—C7—C11	162.50 (10)
C1—N3—C2—N1	0.91 (12)	C5—C7—C8—C9	−61.13 (13)
C3—N4—C2—N3	179.07 (12)	C14—C7—C8—C9	177.43 (11)
C3—N4—C2—N1	1.30 (17)	C11—C7—C8—C9	60.38 (14)
N2—N1—C2—N3	−0.95 (13)	C7—C8—C9—C10	−118.44 (14)
C5—N1—C2—N3	177.27 (10)	C5—C7—C11—C12	−173.66 (10)
N2—N1—C2—N4	177.22 (10)	C14—C7—C11—C12	−53.73 (14)
C5—N1—C2—N4	−4.56 (18)	C8—C7—C11—C12	64.83 (14)
C2—N4—C3—C4	2.01 (17)	C7—C11—C12—C13	104.71 (15)
C2—N4—C3—C6	−177.65 (11)	C15—O2—C14—O1	5.68 (17)
N4—C3—C4—C5	−2.33 (18)	C15—O2—C14—C7	−179.35 (9)
C6—C3—C4—C5	177.32 (12)	C5—C7—C14—O1	−139.28 (12)
C3—C4—C5—N1	−0.75 (17)	C8—C7—C14—O1	−18.80 (16)
C3—C4—C5—C7	−177.85 (11)	C11—C7—C14—O1	101.79 (13)
N2—N1—C5—C4	−178.06 (11)	C5—C7—C14—O2	45.70 (13)
C2—N1—C5—C4	4.03 (16)	C8—C7—C14—O2	166.19 (9)
N2—N1—C5—C7	−0.71 (17)	C11—C7—C14—O2	−73.23 (11)
C2—N1—C5—C7	−178.61 (10)	C14—O2—C15—C16	80.88 (14)
C4—C5—C7—C14	−137.48 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1^{i}	0.962 (14)	2.315 (14)	3.2388 (15)	160.7 (11)
C16—H16*A*···N4^{ii}	0.976 (16)	2.610 (16)	3.4354 (18)	142.4 (12)
C12—H12···*Cg*1^{iii}	0.981 (15)	2.955 (15)	3.6559 (15)	129.3 (11)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) −*x*+3/2, *y*+1/2, −*z*+3/2; (iii) −*x*+1/2, *y*+1/2, −*z*+3/2.