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Allyl 6-amino-5-cyano-2-methyl-4-phenyl-4*H*-pyran-3-carboxylate

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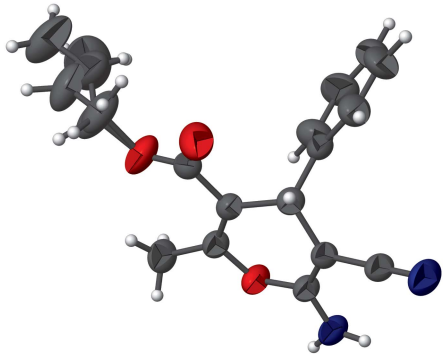
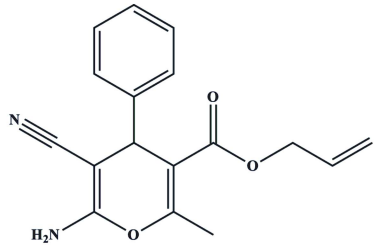
In the title compound, $C_{17}H_{16}N_2O_3$, the 4*H*-pyran ring adopts a boat conformation. In the crystal, N—H···N and N—H···O interactions link the molecules, forming an infinite ribbon running along the *a*-axis direction with N—H···N interactions forming centrosymmetric $R_2^2(12)$ graph-set motifs. The allyl side chain is disordered over two sets of sites with occupancies of 0.720 (7) and 0.280 (7).

3D view



Chemical scheme



Structure description

Pyran derivatives constitute a useful class of heterocyclic compounds, which are widely distributed in nature (Moriguchi *et al.*, 1997). A number of 2-amino-4*H*-pyrans are used as photoactive materials (Armesto *et al.*, 1989), pigments (Rideout *et al.*, 1976) and potentially biodegradable agrochemicals (Kumar *et al.*, 2009). Substituted allyl 6-amino-4*H*-pyran derivatives exhibit a wide range of biological properties including anti-proliferative and antitubercular activities (Panda *et al.*, 1997; Mungra *et al.*, 2011) and 4*H*-pyran derivatives are widely used as organic intermediates (Liang *et al.*, 2009).

The 4*H*-pyran ring in the title compound (Fig. 1) exhibits a boat conformation with puckering parameters Q = 0.230 (3) Å, θ = 79.8 (7)° and φ = 191.1 (7)°. In this ring, the atoms O1 and C7 make the largest deviations of 0.118 (2) and 0.139 (2) Å, respectively, from the mean plane. The C7—C8—C9—C13 and C7—C11—C10—N1 torsion angles are 179.3 (2) and 171.0 (2)°, respectively. The dihedral angle between 4*H*-pyran ring and the phenyl ring is 85.51 (15)°. The bond lengths in the 4*H*-pyran ring are similar to those in a

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···N2^{i}	0.83 (2)	2.24 (2)	3.051 (2)	166.0 (19)
N1—H1*N*2···O2^{ii}	0.88 (2)	2.04 (2)	2.919 (2)	171 (2)
C13—H13*A*···O3	0.96	2.27	2.868 (3)	120

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

related compound (Mohandas *et al.*, 2015). An intramolecular C—H···O hydrogen bond occurs.

In the crystal, N—H···N and N—H···O interactions (Table 1) link the molecules, forming an infinite ribbon running along [100] (Fig. 2). The N—H···N interactions form an $R_2^2(12)$ graph-set motif.

Synthesis and crystallization

A mixture of benzaldehyde (1.0 mmol), malononitrile (1.0 mmol), allyl 3-oxobutanoate (1.0 mmol) and a few drops of piperidine was stirred magnetically in 30 ml of absolute ethanol at 80°C for 90 min. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was allowed to cool to room temperature and the solvent was evaporated. The resulting solid was collected and washed with cold water and recrystallized from ethanol to obtain the pure product (yield 86%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The allyl side chain is disordered and was refined as having two equivalent conformations with occupancies of 0.720 (7) and 0.280 (7).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{16}N_2O_3$
M_r	296.32
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	8.2151 (5), 9.2850 (5), 11.6086 (7)
α, β, γ (°)	108.184 (4), 103.004 (4), 105.089 (2)
V (Å^3)	765.64 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.20 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.956, 0.960
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3789, 3789, 2207
R_{int}	0.053
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.160, 1.02
No. of reflections	3789
No. of parameters	237
No. of restraints	79
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.28

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2008), *SHELXS* and *SHELXL97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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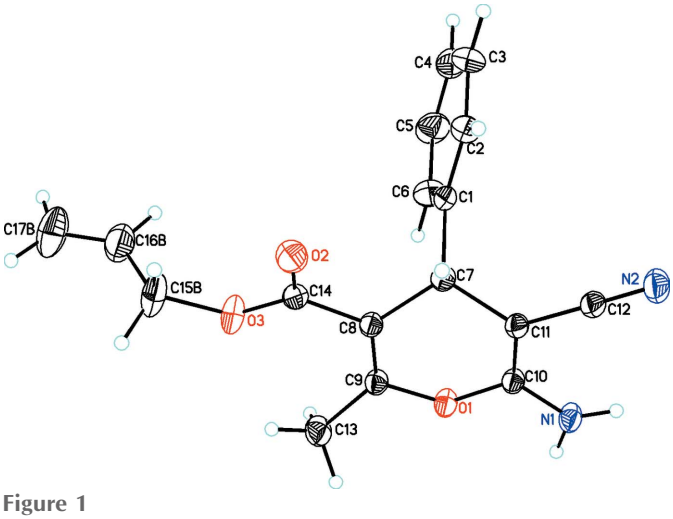

Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 20% probability level (only the major disorder component of the allyl side chain is shown).

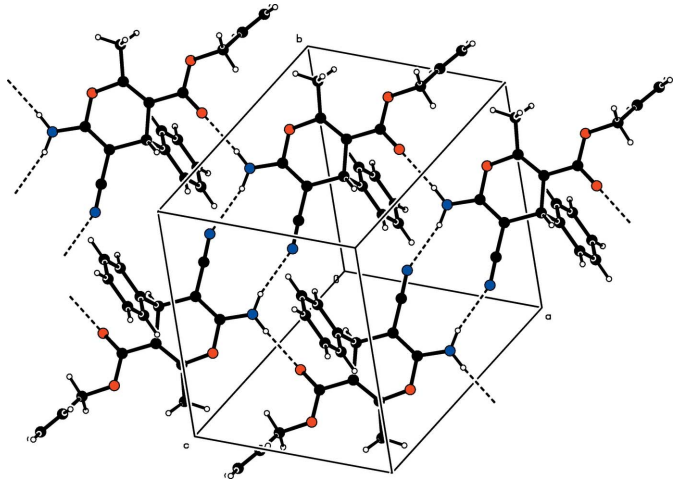

Figure 2
The packing of the title compound (major disorder component only). N—H···N and N—H···O interactions (Table 1) are shown as dashed lines.

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full crystallographic data

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Crystal data

$C_{17}H_{16}N_2O_3$
M_r = 296.32
Triclinic, $P\overline{1}$
a = 8.2151 (5) Å
b = 9.2850 (5) Å
c = 11.6086 (7) Å
α = 108.184 (4)°
β = 103.004 (4)°
γ = 105.089 (2)°
V = 765.64 (8) Å^3
Z = 2
$F(000)$ = 312
D_x = 1.285 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4207 reflections
θ = 2.5–23.4°
μ = 0.09 mm^{-1}
T = 293 K
BLOCK, orange
0.20 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.956, T_{max} = 0.960
3789 measured reflections
3789 independent reflections
2207 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 28.3°, θ_{min} = 2.5°
h = −10→10
k = −12→12
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.160
S = 1.02
3789 reflections
237 parameters
79 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 0.1156P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Extinction correction: SHELXL-2018/3 (Sheldrick 2018), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.028 (6)

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.

Refinement. The positions of the hydrogen atoms bound to the O and C atoms are identified from the difference electron density maps and their distances are geometrically optimized. The hydrogen atoms bound to the C atoms are treated as riding atoms, with d(C—H) = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, d(C—H) = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene and d(C—H) = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl groups. The amine protons were refined isotropically.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.13227 (16)	0.88787 (15)	0.32279 (13)	0.0513 (4)	
O2	0.72395 (18)	0.92452 (18)	0.36162 (17)	0.0742 (5)	
O3	0.62148 (18)	1.06948 (19)	0.26548 (15)	0.0728 (5)	
N1	−0.0492 (2)	0.7331 (2)	0.38698 (18)	0.0580 (5)	
H1N1	−0.080 (3)	0.663 (3)	0.4157 (19)	0.057 (6)*	
H1N2	−0.109 (3)	0.797 (3)	0.376 (2)	0.068 (6)*	
N2	0.1936 (2)	0.4855 (2)	0.48236 (19)	0.0700 (6)	
C1	0.3644 (2)	0.5954 (2)	0.21556 (18)	0.0474 (4)	
C2	0.4475 (3)	0.4852 (3)	0.2186 (2)	0.0693 (6)	
H2A	0.523004	0.495812	0.296026	0.083*	
C3	0.4174 (4)	0.3571 (3)	0.1044 (3)	0.0938 (9)	
H3A	0.472222	0.281595	0.106231	0.113*	
C4	0.3083 (5)	0.3415 (3)	−0.0102 (3)	0.0942 (9)	
H4A	0.290072	0.256420	−0.085936	0.113*	
C5	0.2271 (4)	0.4499 (3)	−0.0129 (2)	0.0881 (8)	
H5A	0.152576	0.439516	−0.090676	0.106*	
C6	0.2543 (3)	0.5753 (3)	0.0988 (2)	0.0700 (6)	
H6A	0.196780	0.648748	0.095559	0.084*	
C7	0.3897 (2)	0.7335 (2)	0.33875 (16)	0.0424 (4)	
H7A	0.494936	0.744799	0.405599	0.051*	
C8	0.4222 (2)	0.8932 (2)	0.32389 (16)	0.0421 (4)	
C9	0.2989 (2)	0.9618 (2)	0.31696 (17)	0.0454 (4)	
C10	0.1074 (2)	0.7670 (2)	0.36705 (16)	0.0437 (4)	
C11	0.2308 (2)	0.6973 (2)	0.38400 (16)	0.0426 (4)	
C12	0.2067 (2)	0.5791 (2)	0.43693 (18)	0.0488 (4)	
C13	0.3033 (3)	1.1169 (3)	0.3039 (2)	0.0652 (6)	
H13A	0.425021	1.184266	0.324493	0.098*	
H13B	0.251375	1.171848	0.361704	0.098*	
H13C	0.236508	1.094610	0.217107	0.098*	
C14	0.6031 (2)	0.9636 (2)	0.31985 (18)	0.0484 (4)	
C15A	0.814 (5)	1.136 (3)	0.2707 (18)	0.084 (3)	0.280 (7)
H15A	0.885611	1.222435	0.354245	0.101*	0.280 (7)
H15B	0.864085	1.051113	0.257234	0.101*	0.280 (7)
C16A	0.8150 (18)	1.1965 (15)	0.1739 (11)	0.098 (3)	0.280 (7)
H16A	0.885497	1.304306	0.198254	0.117*	0.280 (7)
C17A	0.728 (2)	1.1155 (18)	0.0576 (11)	0.149 (5)	0.280 (7)
H17A	0.656193	1.007380	0.029871	0.179*	0.280 (7)
H17B	0.734994	1.163255	−0.001548	0.179*	0.280 (7)
C15B	0.7942 (19)	1.1526 (13)	0.2641 (6)	0.093 (2)	0.720 (7)

H15C	0.824470	1.268629	0.307193	0.111*	0.720 (7)
H15D	0.882796	1.122081	0.311836	0.111*	0.720 (7)
C16B	0.8014 (7)	1.1178 (6)	0.1398 (4)	0.1014 (17)	0.720 (7)
H16B	0.721066	1.016544	0.079943	0.122*	0.720 (7)
C17B	0.8942 (6)	1.1959 (7)	0.0949 (5)	0.1199 (19)	0.720 (7)
H17C	0.978344	1.298620	0.147859	0.144*	0.720 (7)
H17D	0.880257	1.152447	0.007964	0.144*	0.720 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0444 (7)	0.0617 (8)	0.0695 (9)	0.0266 (6)	0.0260 (6)	0.0421 (7)
O2	0.0458 (8)	0.0656 (9)	0.1176 (13)	0.0250 (7)	0.0311 (8)	0.0375 (9)
O3	0.0517 (8)	0.0913 (11)	0.0830 (10)	0.0102 (7)	0.0273 (7)	0.0531 (9)
N1	0.0509 (10)	0.0682 (12)	0.0831 (13)	0.0301 (9)	0.0369 (9)	0.0483 (10)
N2	0.0740 (12)	0.0741 (12)	0.0988 (15)	0.0377 (10)	0.0476 (11)	0.0585 (12)
C1	0.0468 (10)	0.0454 (10)	0.0596 (11)	0.0179 (8)	0.0293 (9)	0.0237 (9)
C2	0.0816 (15)	0.0599 (13)	0.0913 (16)	0.0384 (12)	0.0465 (13)	0.0384 (12)
C3	0.127 (2)	0.0589 (15)	0.127 (3)	0.0528 (16)	0.078 (2)	0.0362 (16)
C4	0.123 (2)	0.0610 (16)	0.090 (2)	0.0183 (16)	0.0658 (19)	0.0093 (14)
C5	0.0939 (19)	0.0846 (18)	0.0627 (15)	0.0207 (15)	0.0283 (13)	0.0073 (13)
C6	0.0752 (14)	0.0731 (15)	0.0587 (13)	0.0329 (12)	0.0226 (11)	0.0165 (11)
C7	0.0400 (9)	0.0474 (10)	0.0465 (10)	0.0199 (7)	0.0155 (7)	0.0228 (8)
C8	0.0421 (9)	0.0431 (9)	0.0429 (9)	0.0140 (7)	0.0165 (7)	0.0185 (8)
C9	0.0454 (10)	0.0489 (10)	0.0490 (10)	0.0179 (8)	0.0190 (8)	0.0252 (8)
C10	0.0441 (10)	0.0476 (10)	0.0464 (10)	0.0174 (8)	0.0192 (8)	0.0236 (8)
C11	0.0473 (10)	0.0440 (9)	0.0460 (10)	0.0201 (8)	0.0208 (8)	0.0229 (8)
C12	0.0496 (10)	0.0516 (11)	0.0595 (11)	0.0246 (8)	0.0273 (9)	0.0285 (9)
C13	0.0675 (13)	0.0634 (13)	0.0876 (16)	0.0319 (11)	0.0333 (12)	0.0467 (12)
C14	0.0458 (10)	0.0440 (10)	0.0512 (10)	0.0131 (8)	0.0194 (8)	0.0135 (8)
C15A	0.057 (5)	0.109 (5)	0.094 (5)	0.010 (4)	0.030 (4)	0.061 (4)
C16A	0.076 (4)	0.110 (5)	0.105 (5)	0.001 (5)	0.027 (4)	0.069 (4)
C17A	0.191 (10)	0.144 (8)	0.111 (6)	0.050 (8)	0.035 (8)	0.067 (7)
C15B	0.060 (4)	0.118 (3)	0.084 (2)	−0.006 (3)	0.029 (2)	0.047 (2)
C16B	0.093 (3)	0.098 (3)	0.096 (3)	0.007 (3)	0.049 (2)	0.027 (3)
C17B	0.095 (3)	0.175 (5)	0.099 (3)	0.018 (3)	0.042 (2)	0.085 (3)

Geometric parameters (Å, º)

O1—C10	1.361 (2)	C7—H7A	0.9800
O1—C9	1.389 (2)	C8—C9	1.331 (2)
O2—C14	1.197 (2)	C8—C14	1.477 (2)
O3—C14	1.319 (2)	C9—C13	1.486 (2)
O3—C15B	1.434 (13)	C10—C11	1.348 (2)
O3—C15A	1.52 (4)	C11—C12	1.409 (2)
N1—C10	1.333 (2)	C13—H13A	0.9600
N1—H1N1	0.83 (2)	C13—H13B	0.9600
N1—H1N2	0.88 (2)	C13—H13C	0.9600

N2—C12	1.143 (2)	C15A—C16A	1.404 (4)
C1—C2	1.375 (3)	C15A—H15A	0.9700
C1—C6	1.376 (3)	C15A—H15B	0.9700
C1—C7	1.521 (2)	C16A—C17A	1.245 (4)
C2—C3	1.396 (4)	C16A—H16A	0.9300
C2—H2A	0.9300	C17A—H17A	0.9300
C3—C4	1.367 (4)	C17A—H17B	0.9300
C3—H3A	0.9300	C15B—C16B	1.395 (4)
C4—C5	1.349 (4)	C15B—H15C	0.9700
C4—H4A	0.9300	C15B—H15D	0.9700
C5—C6	1.371 (3)	C16B—C17B	1.227 (3)
C5—H5A	0.9300	C16B—H16B	0.9300
C6—H6A	0.9300	C17B—H17C	0.9300
C7—C8	1.508 (2)	C17B—H17D	0.9300
C7—C11	1.511 (2)		

C10—O1—C9	119.93 (13)	C11—C10—O1	121.05 (15)
C14—O3—C15B	120.1 (4)	C10—C11—C12	119.89 (15)
C14—O3—C15A	110.7 (7)	C10—C11—C7	121.69 (15)
C10—N1—H1N1	120.4 (14)	C12—C11—C7	118.27 (14)
C10—N1—H1N2	116.0 (14)	N2—C12—C11	177.5 (2)
H1N1—N1—H1N2	123 (2)	C9—C13—H13A	109.5
C2—C1—C6	118.3 (2)	C9—C13—H13B	109.5
C2—C1—C7	120.80 (19)	H13A—C13—H13B	109.5
C6—C1—C7	120.86 (16)	C9—C13—H13C	109.5
C1—C2—C3	119.4 (2)	H13A—C13—H13C	109.5
C1—C2—H2A	120.3	H13B—C13—H13C	109.5
C3—C2—H2A	120.3	O2—C14—O3	122.49 (17)
C4—C3—C2	120.8 (2)	O2—C14—C8	121.74 (17)
C4—C3—H3A	119.6	O3—C14—C8	115.75 (16)
C2—C3—H3A	119.6	C16A—C15A—O3	108 (2)
C5—C4—C3	119.7 (2)	C16A—C15A—H15A	110.1
C5—C4—H4A	120.1	O3—C15A—H15A	110.1
C3—C4—H4A	120.1	C16A—C15A—H15B	110.1
C4—C5—C6	120.1 (3)	O3—C15A—H15B	110.1
C4—C5—H5A	120.0	H15A—C15A—H15B	108.4
C6—C5—H5A	120.0	C17A—C16A—C15A	124.5 (11)
C5—C6—C1	121.7 (2)	C17A—C16A—H16A	117.7
C5—C6—H6A	119.1	C15A—C16A—H16A	117.7
C1—C6—H6A	119.1	C16A—C17A—H17A	120.0
C8—C7—C11	109.31 (13)	C16A—C17A—H17B	120.0
C8—C7—C1	112.26 (14)	H17A—C17A—H17B	120.0
C11—C7—C1	111.41 (14)	C16B—C15B—O3	112.7 (8)
C8—C7—H7A	107.9	C16B—C15B—H15C	109.1
C11—C7—H7A	107.9	O3—C15B—H15C	109.1
C1—C7—H7A	107.9	C16B—C15B—H15D	109.1
C9—C8—C14	124.63 (16)	O3—C15B—H15D	109.1
C9—C8—C7	122.28 (15)	H15C—C15B—H15D	107.8

C14—C8—C7	113.08 (15)	C17B—C16B—C15B	131.9 (8)
C8—C9—O1	120.91 (15)	C17B—C16B—H16B	114.0
C8—C9—C13	131.04 (17)	C15B—C16B—H16B	114.0
O1—C9—C13	108.05 (15)	C16B—C17B—H17C	120.0
N1—C10—C11	128.55 (17)	C16B—C17B—H17D	120.0
N1—C10—O1	110.40 (15)	H17C—C17B—H17D	120.0
C6—C1—C2—C3	−0.2 (3)	C9—O1—C10—N1	168.74 (16)
C7—C1—C2—C3	178.11 (18)	C9—O1—C10—C11	−11.9 (2)
C1—C2—C3—C4	0.8 (4)	N1—C10—C11—C12	−4.5 (3)
C2—C3—C4—C5	−0.7 (4)	O1—C10—C11—C12	176.32 (16)
C3—C4—C5—C6	0.1 (4)	N1—C10—C11—C7	171.01 (18)
C4—C5—C6—C1	0.4 (4)	O1—C10—C11—C7	−8.2 (3)
C2—C1—C6—C5	−0.4 (3)	C8—C7—C11—C10	21.4 (2)
C7—C1—C6—C5	−178.71 (19)	C1—C7—C11—C10	−103.26 (19)
C2—C1—C7—C8	135.66 (18)	C8—C7—C11—C12	−163.08 (15)
C6—C1—C7—C8	−46.0 (2)	C1—C7—C11—C12	72.3 (2)
C2—C1—C7—C11	−101.37 (19)	C15B—O3—C14—O2	−5.2 (5)
C6—C1—C7—C11	76.9 (2)	C15A—O3—C14—O2	−2.7 (9)
C11—C7—C8—C9	−17.1 (2)	C15B—O3—C14—C8	176.0 (4)
C1—C7—C8—C9	106.99 (19)	C15A—O3—C14—C8	178.4 (9)
C11—C7—C8—C14	162.07 (14)	C9—C8—C14—O2	158.52 (19)
C1—C7—C8—C14	−73.79 (18)	C7—C8—C14—O2	−20.7 (2)
C14—C8—C9—O1	−179.35 (15)	C9—C8—C14—O3	−22.6 (3)
C7—C8—C9—O1	−0.2 (3)	C7—C8—C14—O3	158.17 (15)
C14—C8—C9—C13	0.1 (3)	C14—O3—C15A—C16A	158.0 (12)
C7—C8—C9—C13	179.25 (19)	O3—C15A—C16A—C17A	−56 (3)
C10—O1—C9—C8	16.3 (2)	C14—O3—C15B—C16B	117.5 (6)
C10—O1—C9—C13	−163.28 (16)	O3—C15B—C16B—C17B	152.6 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···N2^{i}	0.83 (2)	2.24 (2)	3.051 (2)	166.0 (19)
N1—H1*N*2···O2^{ii}	0.88 (2)	2.04 (2)	2.919 (2)	171 (2)
C13—H13*A*···O3	0.96	2.27	2.868 (3)	120

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