Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 2-(2-{[(benzyloxy)carbonyl]-amino}propan-2-yl)-5-hydroxy-6-oxo-1,6-dihydropyrimidine-4-carboxylate

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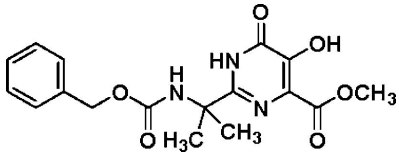
Received 20 March 2011; accepted 29 April 2011

Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.103; data-to-parameter ratio = 16.6.

In the title compound, $C_{17}H_{19}N_3O_6$, the dihedral angle between the two aromatic rings is 45.9 (1)°. The crystal structure is stabilized through intermolecular N—H···O hydrogen bonds and intramolecular O—H···O hydrogen bonds are also present.

Related literature

For related structures, see: Fun *et al.* (2009); Shang & Shang (2007). The title compound is an intermediate in the preparation of the antiretroviral drug raltegravir [systematic name *N*-(2-(4-(4-fluorobenzylcarbamoyl)-5-hydroxy-1-methyl-6-oxo-1,6-dihydropyrimidin-2-yl)propan-2-yl)-5-methyl-1,3,4-oxadiazole-2-carboxamide. For therapeutic details of raltegravir, see Steigbigel *et al.* (2008). For synthetic details, see: Culbertson (1979).



Experimental

Crystal data

$C_{17}H_{19}N_3O_6$ M_r = 361.35
Monoclinic, $P2_1/c$
a = 12.122 (2) Å
b = 16.300 (3) Å
c = 9.1766 (18) Å
β = 106.29 (3)°
V = 1740.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 113 K
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.975, T_{max} = 0.983
15564 measured reflections
4142 independent reflections
3386 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.09
4142 reflections
250 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O5^{i}	0.882 (15)	2.133 (15)	2.8911 (14)	143.7 (12)
N2—H2···O2^{ii}	0.938 (16)	1.886 (16)	2.8135 (16)	169.3 (13)
O1—H1···O3	0.918 (17)	1.788 (17)	2.6163 (14)	148.7 (16)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the funds of Hebei Province Science and Technology Research and Development Projects (No. 08276409D) and Hebei University of Science and Technology.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2426).

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supporting information

Acta Cryst. (2011). E**67**, o1336 [doi:10.1107/S1600536811016278]

Methyl 2-(2-{[(benzyloxy)carbonyl]amino}propan-2-yl)-5-hydroxy-6-oxo-1,6-dihydropyrimidine-4-carboxylate

Zhenhua Shang, Jing Ha, Yifeng Yu and Xiaodan Zhao

S1. Comment

Raltegravir (MK-0518, brand name Isentress), an antiretroviral drug produced by Merck & Co, is used to treat HIV infection (Steigbigel *et al.*, 2008). It received FDA approval in October 2007, the first of a new class of HIV drugs, the integrase inhibitors, to receive such approval. The title compound is a key intermediate in the preparation of Raltegravir.

The pyrimidinone ring is planar, as it is in a related compound (Fun *et al.*, 2009). This is in contrast with another related compound (Shang *et al.*, 2007), where the heterocyclic ring is twisted. In the title compound the dihedral angle between the two aromatic rings is 45.9 (1)°. The crystal structure is stabilized through intermolecular N—H···O hydrogen bonds; intramolecular O—H···O hydrogen bonds are also present.

S2. Experimental

The title compound was prepared by a published method (Culbertson, 1979). To a slurry of benzyl 1-amino-1-(hydroxyimino)-2-methylpropan-2-ylcarbamate (2.9 g) in methanol (12 ml) was added dimethyl acetylenedicarboxylate (1.77 g) slowly at room temperature. After 1.5 h, the mixture was added to xylene (20 ml). The reaction mixture was then heated to reflux for 2 h and cooled to 60 °C. Methyl tert-butyl ether (9 ml) was added slowly to build a seed bed. The batch was then cooled to 0 °C for 14 h, and then further cooled to -5 °C and allowed to stand for 1 h before filtration. The solid was washed with methyl tert-butyl ether (4 ml) and dried. 50 mg of the title compound was dissolved in 30 ml methanol and the solution was kept at room temperature for 10 d. Natural evaporation gave colorless single crystals of the title compound which were suitable for X-ray analysis.

S3. Refinement

All H atoms attached to C atoms were positioned geometrically and treated as riding with C—H = 0.95 Å (aromatic), 0.98 Å (methyl group) and 0.99 Å (methyene group). U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and 1.2 for all other carbon-bound H atoms. The positional parameters of the nitrogen-bound H and oxygen-bound H atoms were refined freely (N—H = 0.882 (15) and 0.938 (16) Å; O—H = 0.918 (17) Å).

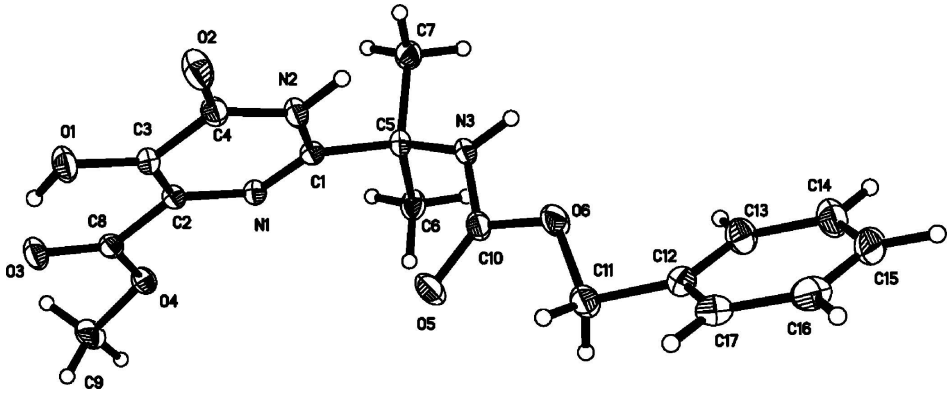

Figure 1

The molecular structure of the title compound, drawn with 30% probability ellipsoids. Hydrogen atoms are shown as spheres of arbitrary radius.

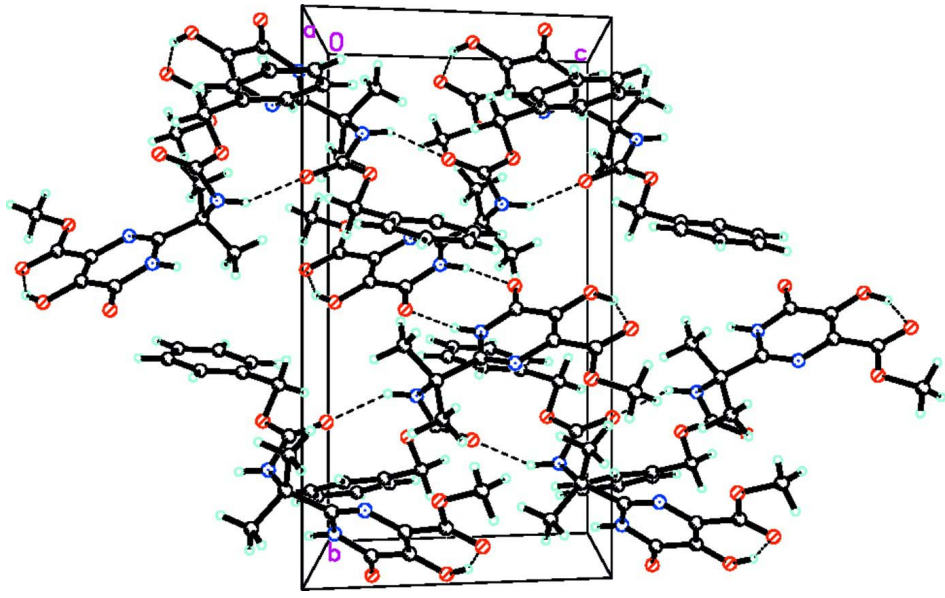

Figure 2

The packing of the title compound,viewed down the *a* axis. The dashed lines indicate the hydrogen bonds.

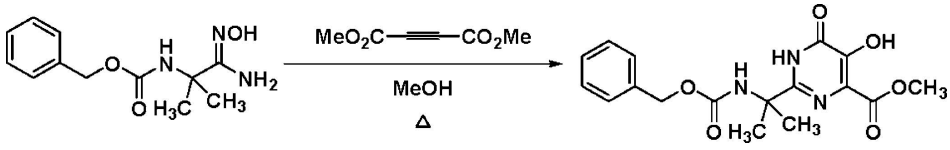

Figure 3

The formation of the title compound.

Methyl 2-(2-{[(benzyloxy)carbonyl]amino}propan-2-yl)-5-hydroxy- 6-oxo-1,6-dihydropyrimidine-4-carboxylate

Crystal data

$C_{17}H_{19}N_3O_6$
M_r = 361.35
Monoclinic, $P2_1/c$
a = 12.122 (2) Å
b = 16.300 (3) Å
c = 9.1766 (18) Å

β = 106.29 (3)°
V = 1740.4 (6) Å^3
Z = 4
F(000) = 760
D_x = 1.379 Mg m^{-3}
Melting point = 183–185 K
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 4990 reflections
θ = 2.5–27.9°
μ = 0.11 mm^{-1}
T = 113 K
Plate, colorless
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART diffractometer
Radiation source: rotating anode
Confocal monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.975, T_{max} = 0.983

15564 measured reflections
4142 independent reflections
3386 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.9°, θ_{min} = 2.5°
h = −15→15
k = −21→18
l = −11→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.09
4142 reflections
250 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.1964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Special details

Experimental. 1*H*-NMR (500 MHz, DMSO) 1.51(s, 6H), 3.82(s, 3H), 4.98(s, 2H), 7.35(bs, 5H), 7.45 (s, 1H), 10.24(s, 1H), 12.58(s, 1H)

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.18567 (8)	0.11941 (5)	0.81459 (10)	0.0159 (2)
N2	0.36822 (8)	0.06461 (6)	0.92786 (11)	0.0179 (2)
N3	0.39582 (8)	0.18366 (6)	1.15086 (11)	0.0170 (2)
O1	0.28432 (8)	−0.00917 (5)	0.54614 (9)	0.0247 (2)
O2	0.45987 (7)	−0.02265 (5)	0.80609 (9)	0.0282 (2)
O3	0.08230 (7)	0.05655 (5)	0.42611 (9)	0.0234 (2)
O4	0.01176 (7)	0.14406 (5)	0.56692 (9)	0.01951 (19)

O5	0.40819 (7)	0.26902 (6)	0.95868 (9)	0.0279 (2)
O6	0.54363 (7)	0.26725 (5)	1.18631 (10)	0.0285 (2)
C1	0.27523 (9)	0.11186 (6)	0.93025 (12)	0.0148 (2)
C2	0.18776 (9)	0.07855 (6)	0.68378 (12)	0.0160 (2)
C3	0.27744 (10)	0.03116 (7)	0.67123 (12)	0.0176 (2)
C4	0.37656 (10)	0.02098 (7)	0.80389 (13)	0.0196 (2)
C5	0.27947 (9)	0.15246 (6)	1.08134 (12)	0.0157 (2)
C6	0.18968 (10)	0.22037 (7)	1.05981 (14)	0.0215 (3)
H6A	0.1929	0.2448	1.1585	0.032*
H6B	0.1130	0.1973	1.0147	0.032*
H6C	0.2055	0.2626	0.9924	0.032*
C7	0.25766 (11)	0.08712 (7)	1.18957 (13)	0.0216 (3)
H7A	0.3156	0.0437	1.2026	0.032*
H7B	0.1810	0.0635	1.1472	0.032*
H7C	0.2624	0.1122	1.2882	0.032*
C8	0.08872 (9)	0.09093 (7)	0.54685 (12)	0.0171 (2)
C9	−0.07754 (10)	0.16603 (8)	0.43090 (14)	0.0259 (3)
H9A	−0.0423	0.1845	0.3526	0.039*
H9B	−0.1245	0.2103	0.4542	0.039*
H9C	−0.1262	0.1181	0.3938	0.039*
C10	0.44448 (10)	0.24266 (7)	1.08715 (13)	0.0185 (2)
C11	0.60365 (11)	0.33419 (8)	1.13972 (14)	0.0266 (3)
H11A	0.5518	0.3818	1.1074	0.032*
H11B	0.6333	0.3173	1.0541	0.032*
C12	0.70133 (10)	0.35578 (7)	1.27658 (13)	0.0206 (3)
C13	0.68387 (11)	0.36043 (8)	1.41951 (14)	0.0247 (3)
H13	0.6100	0.3491	1.4314	0.030*
C14	0.77345 (11)	0.38150 (8)	1.54519 (15)	0.0284 (3)
H14	0.7609	0.3838	1.6427	0.034*
C15	0.88144 (11)	0.39923 (8)	1.52900 (16)	0.0302 (3)
H15	0.9424	0.4144	1.6149	0.036*
C16	0.89961 (11)	0.39465 (8)	1.38730 (16)	0.0282 (3)
H16	0.9733	0.4067	1.3755	0.034*
C17	0.80992 (10)	0.37236 (7)	1.26174 (15)	0.0230 (3)
H17	0.8232	0.3685	1.1648	0.028*
H3	0.4221 (12)	0.1800 (8)	1.2505 (17)	0.024 (3)*
H2	0.4269 (13)	0.0577 (9)	1.0186 (18)	0.036 (4)*
H1	0.2178 (15)	0.0049 (10)	0.474 (2)	0.045 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0170 (5)	0.0159 (4)	0.0139 (4)	−0.0015 (3)	0.0029 (4)	−0.0008 (3)
N2	0.0177 (5)	0.0210 (5)	0.0134 (4)	0.0034 (4)	0.0014 (4)	−0.0024 (4)
N3	0.0182 (5)	0.0189 (5)	0.0116 (4)	−0.0021 (4)	0.0004 (4)	−0.0005 (4)
O1	0.0292 (5)	0.0293 (5)	0.0143 (4)	0.0056 (4)	0.0038 (4)	−0.0051 (3)
O2	0.0265 (5)	0.0372 (5)	0.0188 (4)	0.0140 (4)	0.0029 (4)	−0.0049 (4)
O3	0.0259 (5)	0.0283 (4)	0.0135 (4)	−0.0018 (3)	0.0012 (3)	−0.0026 (3)

O4	0.0173 (4)	0.0220 (4)	0.0158 (4)	0.0007 (3)	−0.0010 (3)	0.0012 (3)
O5	0.0294 (5)	0.0371 (5)	0.0142 (4)	−0.0095 (4)	0.0009 (3)	0.0056 (4)
O6	0.0273 (5)	0.0334 (5)	0.0189 (4)	−0.0152 (4)	−0.0031 (4)	0.0055 (4)
C1	0.0154 (5)	0.0143 (5)	0.0147 (5)	−0.0011 (4)	0.0040 (4)	0.0004 (4)
C2	0.0180 (6)	0.0156 (5)	0.0129 (5)	−0.0018 (4)	0.0019 (4)	0.0005 (4)
C3	0.0227 (6)	0.0164 (5)	0.0130 (5)	−0.0011 (4)	0.0037 (4)	−0.0015 (4)
C4	0.0220 (6)	0.0202 (6)	0.0158 (5)	0.0029 (4)	0.0040 (4)	−0.0011 (4)
C5	0.0158 (5)	0.0169 (5)	0.0135 (5)	−0.0011 (4)	0.0025 (4)	−0.0028 (4)
C6	0.0209 (6)	0.0212 (6)	0.0209 (6)	0.0033 (4)	0.0034 (5)	−0.0051 (5)
C7	0.0265 (6)	0.0216 (6)	0.0182 (6)	−0.0037 (4)	0.0087 (5)	−0.0015 (4)
C8	0.0183 (6)	0.0171 (5)	0.0149 (5)	−0.0043 (4)	0.0031 (4)	0.0009 (4)
C9	0.0209 (6)	0.0308 (7)	0.0201 (6)	0.0011 (5)	−0.0037 (5)	0.0048 (5)
C10	0.0197 (6)	0.0209 (5)	0.0139 (5)	−0.0017 (4)	0.0030 (4)	−0.0018 (4)
C11	0.0276 (7)	0.0319 (7)	0.0181 (6)	−0.0124 (5)	0.0028 (5)	0.0028 (5)
C12	0.0208 (6)	0.0190 (5)	0.0204 (6)	−0.0025 (4)	0.0034 (5)	0.0002 (4)
C13	0.0195 (6)	0.0305 (6)	0.0230 (6)	−0.0005 (5)	0.0041 (5)	−0.0011 (5)
C14	0.0306 (7)	0.0309 (7)	0.0206 (6)	0.0027 (5)	0.0020 (5)	−0.0040 (5)
C15	0.0239 (6)	0.0263 (6)	0.0317 (7)	−0.0014 (5)	−0.0067 (5)	0.0005 (5)
C16	0.0172 (6)	0.0249 (6)	0.0390 (7)	−0.0007 (5)	0.0019 (5)	0.0080 (6)
C17	0.0236 (6)	0.0202 (6)	0.0262 (6)	0.0016 (4)	0.0084 (5)	0.0042 (5)

Geometric parameters (Å, º)

N1—C1	1.2937 (14)	C6—H6A	0.9800
N1—C2	1.3792 (14)	C6—H6B	0.9800
N2—C4	1.3692 (15)	C6—H6C	0.9800
N2—C1	1.3704 (14)	C7—H7A	0.9800
N2—H2	0.938 (16)	C7—H7B	0.9800
N3—C10	1.3446 (15)	C7—H7C	0.9800
N3—C5	1.4663 (14)	C9—H9A	0.9800
N3—H3	0.882 (15)	C9—H9B	0.9800
O1—C3	1.3456 (14)	C9—H9C	0.9800
O1—H1	0.918 (17)	C11—C12	1.5062 (16)
O2—C4	1.2308 (14)	C11—H11A	0.9900
O3—C8	1.2245 (14)	C11—H11B	0.9900
O4—C8	1.3230 (14)	C12—C17	1.3874 (18)
O4—C9	1.4491 (13)	C12—C13	1.3881 (18)
O5—C10	1.2154 (14)	C13—C14	1.3872 (17)
O6—C10	1.3489 (13)	C13—H13	0.9500
O6—C11	1.4413 (14)	C14—C15	1.389 (2)
C1—C5	1.5242 (15)	C14—H14	0.9500
C2—C3	1.3646 (16)	C15—C16	1.380 (2)
C2—C8	1.4881 (15)	C15—H15	0.9500
C3—C4	1.4602 (16)	C16—C17	1.3924 (18)
C5—C6	1.5259 (15)	C16—H16	0.9500
C5—C7	1.5291 (16)	C17—H17	0.9500
C1—N1—C2	116.87 (10)	H7A—C7—H7C	109.5

C4—N2—C1	123.91 (10)	H7B—C7—H7C	109.5
C4—N2—H2	117.4 (9)	O3—C8—O4	123.86 (10)
C1—N2—H2	118.4 (9)	O3—C8—C2	122.24 (11)
C10—N3—C5	123.00 (9)	O4—C8—C2	113.87 (9)
C10—N3—H3	115.1 (9)	O4—C9—H9A	109.5
C5—N3—H3	116.8 (9)	O4—C9—H9B	109.5
C3—O1—H1	104.1 (11)	H9A—C9—H9B	109.5
C8—O4—C9	115.30 (9)	O4—C9—H9C	109.5
C10—O6—C11	116.95 (9)	H9A—C9—H9C	109.5
N1—C1—N2	123.03 (10)	H9B—C9—H9C	109.5
N1—C1—C5	120.75 (10)	O5—C10—N3	126.23 (11)
N2—C1—C5	116.14 (9)	O5—C10—O6	124.12 (11)
C3—C2—N1	123.81 (10)	N3—C10—O6	109.62 (9)
C3—C2—C8	118.60 (10)	O6—C11—C12	105.89 (9)
N1—C2—C8	117.51 (10)	O6—C11—H11A	110.6
O1—C3—C2	126.16 (10)	C12—C11—H11A	110.6
O1—C3—C4	114.98 (10)	O6—C11—H11B	110.6
C2—C3—C4	118.86 (10)	C12—C11—H11B	110.6
O2—C4—N2	122.55 (10)	H11A—C11—H11B	108.7
O2—C4—C3	123.97 (11)	C17—C12—C13	118.85 (11)
N2—C4—C3	113.48 (10)	C17—C12—C11	120.61 (12)
N3—C5—C1	109.22 (9)	C13—C12—C11	120.53 (11)
N3—C5—C6	111.64 (9)	C14—C13—C12	120.51 (12)
C1—C5—C6	110.88 (9)	C14—C13—H13	119.7
N3—C5—C7	106.23 (9)	C12—C13—H13	119.7
C1—C5—C7	108.70 (9)	C13—C14—C15	120.27 (13)
C6—C5—C7	110.02 (10)	C13—C14—H14	119.9
C5—C6—H6A	109.5	C15—C14—H14	119.9
C5—C6—H6B	109.5	C16—C15—C14	119.59 (12)
H6A—C6—H6B	109.5	C16—C15—H15	120.2
C5—C6—H6C	109.5	C14—C15—H15	120.2
H6A—C6—H6C	109.5	C15—C16—C17	119.98 (12)
H6B—C6—H6C	109.5	C15—C16—H16	120.0
C5—C7—H7A	109.5	C17—C16—H16	120.0
C5—C7—H7B	109.5	C12—C17—C16	120.77 (13)
H7A—C7—H7B	109.5	C12—C17—H17	119.6
C5—C7—H7C	109.5	C16—C17—H17	119.6

C2—N1—C1—N2	−1.36 (16)	N1—C1—C5—C7	102.55 (12)
C2—N1—C1—C5	−178.04 (9)	N2—C1—C5—C7	−74.35 (12)
C4—N2—C1—N1	0.28 (18)	C9—O4—C8—O3	−5.78 (16)
C4—N2—C1—C5	177.10 (10)	C9—O4—C8—C2	171.97 (9)
C1—N1—C2—C3	0.47 (16)	C3—C2—C8—O3	4.06 (17)
C1—N1—C2—C8	−176.14 (10)	N1—C2—C8—O3	−179.15 (10)
N1—C2—C3—O1	−179.23 (10)	C3—C2—C8—O4	−173.74 (10)
C8—C2—C3—O1	−2.66 (18)	N1—C2—C8—O4	3.06 (14)
N1—C2—C3—C4	1.43 (17)	C5—N3—C10—O5	−11.21 (19)
C8—C2—C3—C4	178.00 (10)	C5—N3—C10—O6	170.86 (10)

C1—N2—C4—O2	−178.10 (11)	C11—O6—C10—O5	5.83 (18)
C1—N2—C4—C3	1.58 (16)	C11—O6—C10—N3	−176.18 (10)
O1—C3—C4—O2	−2.06 (18)	C10—O6—C11—C12	173.06 (10)
C2—C3—C4—O2	177.35 (11)	O6—C11—C12—C17	137.37 (11)
O1—C3—C4—N2	178.27 (10)	O6—C11—C12—C13	−43.44 (15)
C2—C3—C4—N2	−2.32 (16)	C17—C12—C13—C14	0.16 (18)
C10—N3—C5—C1	63.17 (13)	C11—C12—C13—C14	−179.05 (11)
C10—N3—C5—C6	−59.82 (14)	C12—C13—C14—C15	0.83 (19)
C10—N3—C5—C7	−179.76 (10)	C13—C14—C15—C16	−0.91 (19)
N1—C1—C5—N3	−141.95 (10)	C14—C15—C16—C17	0.00 (19)
N2—C1—C5—N3	41.15 (12)	C13—C12—C17—C16	−1.07 (17)
N1—C1—C5—C6	−18.51 (14)	C11—C12—C17—C16	178.14 (11)
N2—C1—C5—C6	164.59 (10)	C15—C16—C17—C12	1.00 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O5^{i}	0.882 (15)	2.133 (15)	2.8911 (14)	143.7 (12)
N2—H2···O2^{ii}	0.938 (16)	1.886 (16)	2.8135 (16)	169.3 (13)
O1—H1···O3	0.918 (17)	1.788 (17)	2.6163 (14)	148.7 (16)

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