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Methyl (2*R*)-2-benzamido-2-{[(1*R*)-2-methoxy-2-oxo-1-phenylethyl]amino}acetate

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Keywords: crystal structure; α-aminoacetates; hydrogen bonds; one-dimensional chains.

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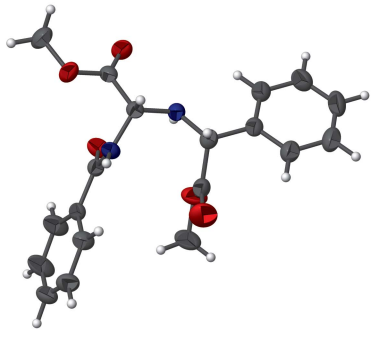
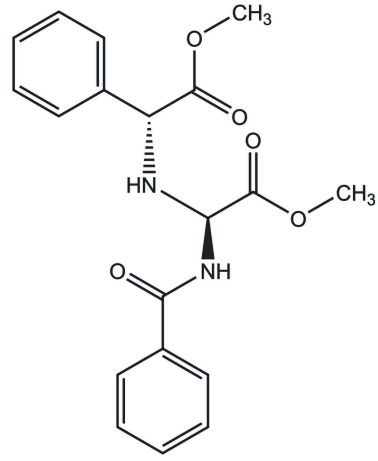
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{19}H_{20}N_2O_5$, the dihedral angle between the phenyl rings is 58.85 (8)°, while that between the planes of the methyl acetate groups is 88.30 (8)°. The molecular conformation is also influenced by the presence of an intramolecular N—H···O hydrogen bond. In the crystal, N—H···O hydrogen bonds link the molecules, forming chains propagating along the *a*-axis direction.

3D view



Chemical scheme



Structure description

The synthesis of new α-AAs (α-aminoacetates) and their esters is of international interest because of their extensive applications in enzymology, medicine, pharmacology and industry (Leite *et al.*, 2006; Mikołajczyk, 2005; Joly *et al.*, 2004). Our strategy used nucleophilic substitution of the *N*-protected methyl α-azido glycinate with 2-amino-2-phenylacetate in methylene chloride, in the presence of triethylamine as a base (Boukallaba *et al.*, 2006) to produce the title compound in good yield.

In the title molecule (Fig. 1), the dihedral angles between the phenyl rings and those between the planes of the methyl acetate groups are 58.85 (8) and 88.30 (8)° respectively. The twisted conformation of the molecule is also influenced by the presence of an intramolecular N—H···O hydrogen bond (Table 1). In the crystal, N—H···O and C—H···O hydrogen bonds (Table 1, Fig. 2) link the molecules into chains propagating along the *a*-axis direction.

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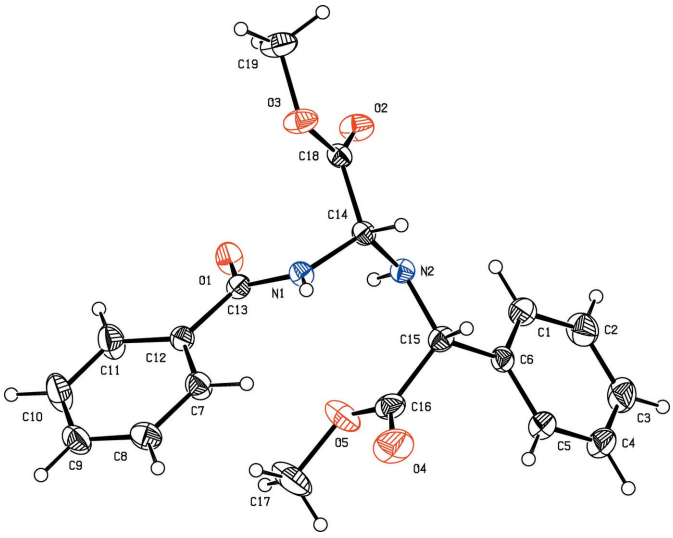

Figure 1
The structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres with arbitrary radii.

Synthesis and crystallization

To a stirred solution of methyl 2-amino-2-phenylacetate (2 mmol) and triethylamine (4 mmol) in 10 ml of dry methylene chloride, *N*-benzoylated methyl α-azidoglycinate (2.6 mmol) was added. The mixture was stirred at 0°C for 1 h then at room temperature for 16 h. The resulting solution was washed with citric acid (15%), then with a saturated solution of sodium bicarbonate ($NaHCO_3$). Solvents were removed and colourless single crystals of the title compound were obtained by recrystallization from ether (yield = 86%; m.p = 126–128°C.).

^{1}H NMR (300.13 MHz; $CDCl_3$, δ_H p.p.m.): 3.3 (*e*, 1H, **NH**–CH–Ph); 3.51 (*s*, 3H, –O**CH$_3$**); 3.78 (*s*, 3H, –O**CH$_3$**); 4.65 (*s*, 1H, NH–**CH**–Ph); 5.52 (*d*, 1H, N–**CH**–N, *J* = 8.4 Hz); 6.75 (*d*, 1H, **NH**Bz, *J* = 8.4 Hz); 7.28–7.82 (*m*, 10H$_{arom}$).

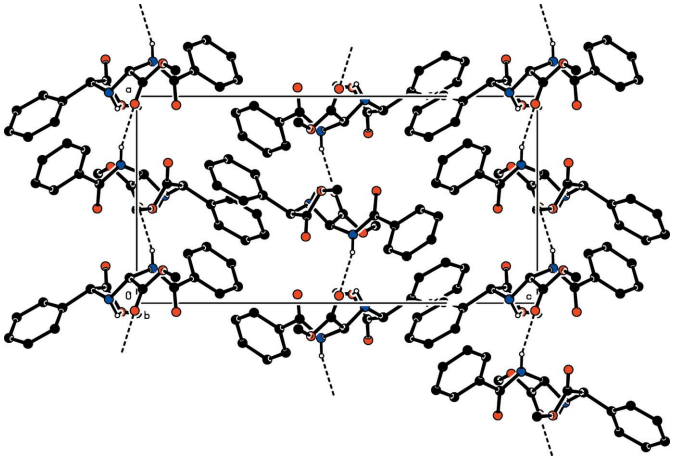

Figure 2
A view of the crystal packing of along the *b* axis. Hydrogen bonds are drawn as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2^{i}	0.85 (1)	2.09 (1)	2.9147 (15)	162 (1)
N2—H2*N*···O5	0.85 (1)	2.52 (1)	2.8334 (15)	103 (1)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{20}N_2O_5$
M_r	356.37
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	173
a, *b*, *c* (Å)	9.3432 (6), 10.4314 (8), 18.0901 (14)
V (Å^3)	1763.1 (2)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.10
Crystal size (mm)	0.35 × 0.16 × 0.14
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2005)
T_{min}, T_{max}	0.967, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28362, 3455, 3246
R_{int}	0.029
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.027, 0.065, 1.04
No. of reflections	3455
No. of parameters	246
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.13
Absolute structure	Flack (1983), 1822 Friedel pairs
Absolute structure parameter	−0.3 (8)

Computer programs: *APEX2* and *SAINT* (Bruker, 2005), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

^{13}C NMR (75.47 MHz; $CDCl_3$, δ_C p.p.m.): 52.44 (1C, O**C**H$_3$); 52.88 (1C, O**C**H$_3$); 61.97 (1C, NH–**C**H—Ph); 63.62 (1C, N–**C**H—N); 127.13–137.48 (10C, **C**$_{arom}$); 167.14, 170.14 and 173.63 (3C, **C**O).

Elemental Analysis: **Calculated** for $C_{19}H_{20}N_2O_5$ (%): C, 64.04; H, 5.66; N, 7.86; **Found** (%): C 63.84, H 5.67, N 7.89. **MS ESI** *m*/*z* (%) = 356.49.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2017). **2**, x171155 [https://doi.org/10.1107/S2414314617011555]

Methyl (2*R*)-2-benzamido-2-{[(1*R*)-2-methoxy-2-oxo-1-phenylethyl]amino}-acetate

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Crystal data

$C_{19}H_{20}N_2O_5$
M_r = 356.37
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 9.3432 (6) Å
b = 10.4314 (8) Å
c = 18.0901 (14) Å
V = 1763.1 (2) Å^3
Z = 4
$F(000)$ = 752
D_x = 1.343 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 365 reflections
θ = 1.6–25.2°
μ = 0.10 mm^{-1}
T = 173 K
Prism, colourless
0.35 × 0.16 × 0.14 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (SADABS; Bruker, 2005)
T_{min} = 0.967, T_{max} = 0.986
28362 measured reflections
3455 independent reflections
3246 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.0°, θ_{min} = 2.3°
h = −11→7
k = −12→12
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.065
S = 1.04
3455 reflections
246 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0234P)^2 + 0.3377P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0073 (8)
Absolute structure: Flack (1983), 1822 Friedel pairs
Absolute structure parameter: −0.3 (8)

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. 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}
C14	0.12279 (14)	0.23661 (11)	0.98202 (7)	0.0305 (3)
H14	0.2102	0.2580	0.9526	0.037*
N1	0.16831 (11)	0.14782 (10)	1.03988 (6)	0.0315 (2)
O3	0.15911 (11)	0.40644 (9)	1.06499 (6)	0.0464 (3)
O1	−0.04242 (10)	0.16104 (10)	1.09856 (6)	0.0456 (3)
O2	−0.03638 (11)	0.41900 (9)	0.99493 (6)	0.0475 (3)
C15	0.06822 (15)	0.08188 (12)	0.88463 (7)	0.0359 (3)
H15	0.1676	0.1036	0.8684	0.043*
N2	0.01902 (12)	0.18778 (10)	0.93039 (6)	0.0321 (2)
C12	0.12463 (14)	0.00585 (12)	1.14380 (7)	0.0330 (3)
C18	0.06847 (13)	0.36261 (11)	1.01468 (7)	0.0323 (3)
C13	0.07640 (13)	0.11150 (12)	1.09329 (7)	0.0322 (3)
C1	−0.12382 (16)	0.15859 (14)	0.79537 (8)	0.0452 (3)
H1	−0.1444	0.2276	0.8279	0.054*
C6	−0.02209 (14)	0.06888 (13)	0.81452 (7)	0.0353 (3)
C9	0.19247 (18)	−0.19864 (15)	1.23588 (9)	0.0493 (4)
H9	0.2146	−0.2693	1.2669	0.059*
O5	−0.04305 (14)	−0.07267 (10)	0.96120 (7)	0.0620 (3)
C8	0.27280 (17)	−0.17514 (15)	1.17398 (9)	0.0479 (4)
H8	0.3519	−0.2288	1.1627	0.057*
C19	0.1260 (2)	0.53040 (15)	1.09662 (10)	0.0572 (4)
H19A	0.1460	0.5977	1.0602	0.086*
H19B	0.1851	0.5443	1.1407	0.086*
H19C	0.0246	0.5332	1.1104	0.086*
C7	0.23931 (16)	−0.07355 (13)	1.12783 (8)	0.0423 (3)
H7	0.2954	−0.0582	1.0849	0.051*
C4	−0.0684 (2)	−0.04241 (16)	0.70022 (9)	0.0571 (4)
H4	−0.0492	−0.1120	0.6678	0.069*
C5	0.00429 (18)	−0.03273 (15)	0.76647 (8)	0.0474 (4)
H5	0.0730	−0.0960	0.7794	0.057*
C11	0.04614 (19)	−0.01734 (17)	1.20718 (9)	0.0560 (4)
H11	−0.0316	0.0373	1.2196	0.067*
C16	0.07709 (18)	−0.04722 (14)	0.92455 (8)	0.0471 (4)
O4	0.17846 (16)	−0.11697 (13)	0.92196 (8)	0.0816 (4)
C3	−0.1684 (2)	0.04823 (18)	0.68102 (9)	0.0619 (5)

H3	−0.2179	0.0418	0.6353	0.074*
C10	0.0801 (2)	−0.11964 (19)	1.25270 (9)	0.0657 (5)
H10	0.0250	−0.1351	1.2959	0.079*
C2	−0.1965 (2)	0.14844 (17)	0.72849 (9)	0.0592 (4)
H2	−0.2660	0.2110	0.7155	0.071*
C17	−0.0486 (3)	−0.19393 (18)	1.00059 (13)	0.0933 (8)
H17A	−0.0225	−0.2637	0.9669	0.140*
H17B	−0.1458	−0.2081	1.0193	0.140*
H17C	0.0186	−0.1918	1.0421	0.140*
H1N	0.2540 (14)	0.1193 (14)	1.0386 (8)	0.039 (4)*
H2N	−0.0591 (14)	0.1679 (13)	0.9516 (7)	0.033 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C14	0.0284 (6)	0.0311 (6)	0.0321 (6)	−0.0018 (5)	−0.0005 (5)	0.0026 (5)
N1	0.0270 (5)	0.0325 (5)	0.0352 (5)	0.0043 (4)	−0.0002 (5)	0.0039 (4)
O3	0.0447 (5)	0.0364 (5)	0.0581 (6)	0.0044 (4)	−0.0181 (5)	−0.0123 (5)
O1	0.0363 (5)	0.0549 (6)	0.0454 (5)	0.0140 (5)	0.0072 (4)	0.0097 (5)
O2	0.0412 (6)	0.0406 (5)	0.0607 (6)	0.0089 (4)	−0.0159 (5)	−0.0052 (5)
C15	0.0341 (6)	0.0374 (7)	0.0362 (7)	−0.0007 (6)	0.0017 (5)	−0.0037 (5)
N2	0.0307 (5)	0.0324 (5)	0.0332 (5)	−0.0013 (4)	−0.0016 (5)	−0.0005 (4)
C12	0.0340 (6)	0.0337 (6)	0.0314 (6)	−0.0010 (5)	−0.0040 (5)	0.0003 (5)
C18	0.0311 (6)	0.0305 (6)	0.0351 (6)	−0.0020 (5)	−0.0040 (5)	0.0042 (5)
C13	0.0322 (6)	0.0333 (6)	0.0310 (6)	0.0022 (5)	−0.0010 (5)	−0.0018 (5)
C1	0.0494 (8)	0.0441 (8)	0.0421 (7)	−0.0024 (7)	−0.0045 (7)	−0.0009 (6)
C6	0.0383 (7)	0.0365 (7)	0.0310 (6)	−0.0076 (5)	0.0033 (5)	0.0012 (5)
C9	0.0577 (9)	0.0423 (8)	0.0479 (8)	−0.0024 (7)	−0.0112 (7)	0.0134 (7)
O5	0.0676 (8)	0.0449 (6)	0.0736 (8)	−0.0110 (6)	−0.0148 (6)	0.0246 (6)
C8	0.0477 (8)	0.0397 (7)	0.0562 (9)	0.0076 (7)	−0.0043 (7)	0.0055 (7)
C19	0.0653 (10)	0.0380 (8)	0.0681 (10)	0.0046 (7)	−0.0147 (9)	−0.0170 (7)
C7	0.0429 (8)	0.0412 (7)	0.0427 (7)	0.0053 (6)	0.0041 (6)	0.0062 (6)
C4	0.0746 (11)	0.0543 (9)	0.0426 (8)	−0.0127 (9)	−0.0008 (8)	−0.0113 (7)
C5	0.0570 (9)	0.0446 (8)	0.0407 (8)	−0.0036 (7)	0.0012 (7)	−0.0050 (7)
C11	0.0566 (10)	0.0626 (10)	0.0487 (8)	0.0169 (8)	0.0150 (8)	0.0159 (8)
C16	0.0599 (9)	0.0377 (7)	0.0436 (8)	0.0078 (7)	−0.0176 (7)	−0.0074 (6)
O4	0.0964 (10)	0.0652 (8)	0.0831 (9)	0.0450 (8)	−0.0142 (8)	−0.0072 (7)
C3	0.0760 (12)	0.0700 (11)	0.0397 (8)	−0.0191 (10)	−0.0167 (8)	0.0003 (8)
C10	0.0731 (12)	0.0746 (12)	0.0494 (9)	0.0129 (10)	0.0160 (9)	0.0265 (9)
C2	0.0636 (10)	0.0595 (10)	0.0546 (10)	−0.0007 (9)	−0.0191 (8)	0.0069 (8)
C17	0.139 (2)	0.0537 (11)	0.0873 (14)	−0.0394 (13)	−0.0489 (15)	0.0349 (10)

Geometric parameters (Å, º)

C14—N2	1.4395 (16)	C9—H9	0.9500
C14—N1	1.4610 (16)	O5—C16	1.331 (2)
C14—C18	1.5277 (17)	O5—C17	1.4527 (19)
C14—H14	1.0000	C8—C7	1.385 (2)

N1—C13	1.3469 (17)	C8—H8	0.9500
N1—H1N	0.855 (13)	C19—H19A	0.9800
O3—C18	1.3246 (15)	C19—H19B	0.9800
O3—C19	1.4474 (17)	C19—H19C	0.9800
O1—C13	1.2282 (15)	C7—H7	0.9500
O2—C18	1.1973 (15)	C4—C3	1.374 (3)
C15—N2	1.4549 (16)	C4—C5	1.381 (2)
C15—C6	1.5294 (18)	C4—H4	0.9500
C15—C16	1.530 (2)	C5—H5	0.9500
C15—H15	1.0000	C11—C10	1.385 (2)
N2—H2N	0.850 (12)	C11—H11	0.9500
C12—C11	1.382 (2)	C16—O4	1.1952 (19)
C12—C7	1.3848 (19)	C3—C2	1.378 (3)
C12—C13	1.5009 (17)	C3—H3	0.9500
C1—C6	1.378 (2)	C10—H10	0.9500
C1—C2	1.392 (2)	C2—H2	0.9500
C1—H1	0.9500	C17—H17A	0.9800
C6—C5	1.393 (2)	C17—H17B	0.9800
C9—C8	1.370 (2)	C17—H17C	0.9800
C9—C10	1.369 (2)		

N2—C14—N1	115.89 (10)	C9—C8—H8	119.8
N2—C14—C18	109.37 (10)	C7—C8—H8	119.8
N1—C14—C18	111.41 (10)	O3—C19—H19A	109.5
N2—C14—H14	106.5	O3—C19—H19B	109.5
N1—C14—H14	106.5	H19A—C19—H19B	109.5
C18—C14—H14	106.5	O3—C19—H19C	109.5
C13—N1—C14	120.44 (11)	H19A—C19—H19C	109.5
C13—N1—H1N	121.3 (10)	H19B—C19—H19C	109.5
C14—N1—H1N	118.2 (10)	C12—C7—C8	120.44 (14)
C18—O3—C19	116.33 (11)	C12—C7—H7	119.8
N2—C15—C6	111.39 (11)	C8—C7—H7	119.8
N2—C15—C16	114.64 (11)	C3—C4—C5	120.22 (16)
C6—C15—C16	110.07 (11)	C3—C4—H4	119.9
N2—C15—H15	106.8	C5—C4—H4	119.9
C6—C15—H15	106.8	C4—C5—C6	120.67 (15)
C16—C15—H15	106.8	C4—C5—H5	119.7
C14—N2—C15	115.15 (10)	C6—C5—H5	119.7
C14—N2—H2N	111.8 (9)	C12—C11—C10	120.44 (15)
C15—N2—H2N	110.0 (10)	C12—C11—H11	119.8
C11—C12—C7	118.61 (13)	C10—C11—H11	119.8
C11—C12—C13	118.31 (12)	O4—C16—O5	124.52 (15)
C7—C12—C13	122.99 (12)	O4—C16—C15	124.07 (16)
O2—C18—O3	123.96 (12)	O5—C16—C15	111.41 (12)
O2—C18—C14	125.39 (12)	C4—C3—C2	119.61 (15)
O3—C18—C14	110.51 (10)	C4—C3—H3	120.2
O1—C13—N1	120.90 (12)	C2—C3—H3	120.2
O1—C13—C12	122.21 (12)	C9—C10—C11	120.49 (15)

N1—C13—C12	116.86 (11)	C9—C10—H10	119.8
C6—C1—C2	120.23 (15)	C11—C10—H10	119.8
C6—C1—H1	119.9	C3—C2—C1	120.43 (16)
C2—C1—H1	119.9	C3—C2—H2	119.8
C1—C6—C5	118.82 (13)	C1—C2—H2	119.8
C1—C6—C15	121.92 (12)	O5—C17—H17A	109.5
C5—C6—C15	119.17 (12)	O5—C17—H17B	109.5
C8—C9—C10	119.61 (14)	H17A—C17—H17B	109.5
C8—C9—H9	120.2	O5—C17—H17C	109.5
C10—C9—H9	120.2	H17A—C17—H17C	109.5
C16—O5—C17	116.64 (16)	H17B—C17—H17C	109.5
C9—C8—C7	120.38 (15)		

N2—C14—N1—C13	−68.46 (15)	N2—C15—C6—C5	−175.99 (12)
C18—C14—N1—C13	57.43 (15)	C16—C15—C6—C5	−47.69 (17)
N1—C14—N2—C15	−64.44 (15)	C10—C9—C8—C7	−1.2 (2)
C18—C14—N2—C15	168.63 (10)	C11—C12—C7—C8	1.0 (2)
C6—C15—N2—C14	−158.86 (11)	C13—C12—C7—C8	−175.46 (13)
C16—C15—N2—C14	75.32 (15)	C9—C8—C7—C12	0.3 (2)
C19—O3—C18—O2	−0.1 (2)	C3—C4—C5—C6	−0.3 (2)
C19—O3—C18—C14	175.61 (13)	C1—C6—C5—C4	1.1 (2)
N2—C14—C18—O2	−7.24 (17)	C15—C6—C5—C4	−175.50 (14)
N1—C14—C18—O2	−136.67 (13)	C7—C12—C11—C10	−1.4 (2)
N2—C14—C18—O3	177.07 (11)	C13—C12—C11—C10	175.25 (16)
N1—C14—C18—O3	47.65 (14)	C17—O5—C16—O4	0.2 (2)
C14—N1—C13—O1	−6.90 (19)	C17—O5—C16—C15	179.10 (13)
C14—N1—C13—C12	171.27 (10)	N2—C15—C16—O4	−131.74 (15)
C11—C12—C13—O1	−13.9 (2)	C6—C15—C16—O4	101.76 (17)
C7—C12—C13—O1	162.54 (13)	N2—C15—C16—O5	49.39 (16)
C11—C12—C13—N1	167.94 (13)	C6—C15—C16—O5	−77.11 (14)
C7—C12—C13—N1	−15.60 (19)	C5—C4—C3—C2	−0.4 (3)
C2—C1—C6—C5	−1.2 (2)	C8—C9—C10—C11	0.8 (3)
C2—C1—C6—C15	175.29 (14)	C12—C11—C10—C9	0.5 (3)
N2—C15—C6—C1	7.55 (18)	C4—C3—C2—C1	0.3 (3)
C16—C15—C6—C1	135.86 (14)	C6—C1—C2—C3	0.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2^{i}	0.85 (1)	2.09 (1)	2.9147 (15)	162 (1)
N2—H2*N*···O5	0.85 (1)	2.52 (1)	2.8334 (15)	103 (1)
C1—H1···N2	0.95	2.44	2.8000 (18)	102
C7—H7···O2^{i}	0.95	2.58	3.4530 (18)	153

Symmetry code: (i) $x+1/2, -y+1/2, -z+2$.