organic compounds

Methyl 2-({6-[(1-methoxy-2-methyl-1-oxopropan-2-yl)carbamoyl]pyridin-2-yl}-formamido)-2-methylpropanoate

Mohamed A. Al-Omar,[a,b] Abdel-Galil E. Amr,[b,c] Hazem A. Ghabbour,[a] Ching Kheng Quah[d]‡ and Hoong-Kun Fun[d]*§

[a]Pharmaceutical Chemistry Department, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia, [b]Drug Exploration & Development Chair (DEDC), College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia, [c]Applied Organic Chemistry Department, National Research Center, Dokki 12622, Cairo, Egypt, and [d]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hkfun@usm.my

In the title compound, $C_{17}H_{23}N_3O_6$, the two methoxycarbonyl C—O—C=O planes are inclined at dihedral angles of 5.3 (4) and 83.9 (4)° with respect to the central pyridine ring. An intramolecular N—H⋯O hydrogen bond generates an $S(5)$ ring motif. In the crystal, molecules are linked into a chain along the c axis *via* C—H⋯O hydrogen bonds.

Related literature

For general background to and the pharmacological activity of the title compound, see: Abou-Ghalia & Amr (2004); Abou-Ghalia *et al.* (2003); Al-Omar & Amr (2010); Amr (2000); Attia *et al.* (1997, 2000); Amr *et al.* (2009); Fakhr *et al.* (2008). For standard bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).

Experimental

Crystal data

$C_{17}H_{23}N_3O_6$	V = 1965.8 (4) Å^3
M_r = 365.38	Z = 4
Orthorhombic, $Pca2_1$	Cu $K\alpha$ radiation
a = 10.2307 (10) Å	μ = 0.79 mm^{-1}
b = 9.3038 (11) Å	T = 296 K
c = 20.652 (2) Å	$0.63 \times 0.52 \times 0.09$ mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	7477 measured reflections
	1898 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	1249 reflections with $I > 2\sigma(I)$
T_{min} = 0.560, T_{max} = 0.932	R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.133	
S = 0.91	
1898 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
250 parameters	$\Delta\rho_{min}$ = -0.17 e Å^{-3}
1 restraint	

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H1$N2$⋯O2	0.85 (4)	2.08 (4)	2.614 (5)	120 (3)
C3—H3A⋯O6^i	0.93	2.49	3.204 (6)	134

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

References

Abou-Ghalia, M. H. & Amr, A. E. (2004). *Amino Acids*, **26**, 283–289.
Abou-Ghalia, M. H., Amr, A. E. & Abdulla, M. M. (2003). *Z. Naturforsch. Teil B*, **58**, 903–910.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Al-Omar, M. A. & Amr, A. E. (2010). *Molecules*, **15**, 4711–4721.
Amr, A. E. (2000). *Indian J. Heterocycl. Chem.* **10**, 49–58.
Amr, A. E., Sabrry, N. M., Abdalla, M. M. & Abdel-Wahab, B. F. (2009). *Eur. J. Med. Chem.* **44**, 725–735.
Attia, A., Abdel-Salam, O. I. & Amr, A. E. (1997). *Egypt. J. Chem.* **40**, 317–325.
Attia, A., Abdel-Salam, O. I. & Amr, A. E. (2000). *Egypt. J. Chem.* **43**, 297–307.

‡ Thomson Reuters ResearcherID: A-5525-2009.
§ Thomson Reuters ResearcherID: A-3561-2009.

organic compounds

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Fakhr, I. M., Amr, A. E., Sabry, N. M. & Abdalah, M. M. (2008). *Arch. Pharm. Chem. Life Sci.* **341**, 174–180.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Methyl 2-({6-[(1-methoxy-2-methyl-1-oxopropan-2-yl)carbamoyl]pyridin-2-yl}formamido)-2-methylpropanoate

Mohamed A. Al-Omar, Abdel-Galil E. Amr, Hazem A. Ghabbour, Ching Kheng Quah and Hoong-Kun Fun

Comment

In our previous work, we have reported that certain substituted pyridines and Schiff base derivatives are antimicrobial, anti-inflammatory and anticancer agents (Abou-Ghalia & Amr, 2004; Abou-Ghalia *et al.*, 2003; Al-Omar & Amr, 2010; Amr, 2000; Attia *et al.*, 1997, 2000). In continuation of our interests in the chemical and pharmacological properties of disubstituted pyridine derivatives (Amr *et al.*, 2009; Fakhr *et al.*, 2008), we report herein the synthesis and antimicrobial activities of the title compound.

In the title molecule (Fig. 1), the two methoxycarbonyl moieties (O2/O3/C8/C9 and O5/O6/C14/C15) are nearly planar [maximum deviations of 0.005 (5) and 0.009 (5) Å at atoms C8 and C14, respectively] and are inclined at angles of 5.3 (4) and 83.9 (4)° with the pyridine ring (N1/C1–C5). Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The molecular structure is stabilized by an intramolecular N2—H1N2···O2 hydrogen bond (Table 1), which generates an *S*(5) ring motif (Bernstein *et al.*, 1995).

In the crystal (Fig. 2), molecules are linked into one-dimensional chains propagating along the [001] direction *via* intermolecular C3—H3A···O6 hydrogen bonds (Table 1).

Experimental

To a solution of 2-methylalanine methyl esters (2 mmol), 2,6-pyridinedicarboyl dichloride (1 mmol) in dichloromethane (15 mL) was added at -10 °C with stirring. Triethylamine was added drop wise to the reaction mixture in order to keep the reaction mixture slightly basic (pH ~ 8). Stirring was continued for 3 h more at -15 °C and then 12 h at r.t. The reaction mixture was then washed with water, 1N hydrochloric acid, 1N sodium bicarbonate and finally with water and dried over anhydrous calcium chloride. The solvent was evaporated under reduced pressure to dryness and the obtained solid was crystallized from chloroform to give the titled bis-ester.

Refinement

Atoms H1N2 and H1N3 were located in a difference Fourier map and refined freely [N—H = 0.84 (4) and 0.95 (5) Å]. The remaining hydrogen atoms were positioned geometrically (C—H = 0.93 or 0.96 Å) and were refined using a riding model, with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C). A rotating group model was applied to the methyl groups. Even though Cu radiation was used, there was not enough anomalous dispersion to determine the absolute configuration. Thus, Friedel pairs have been merged.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).
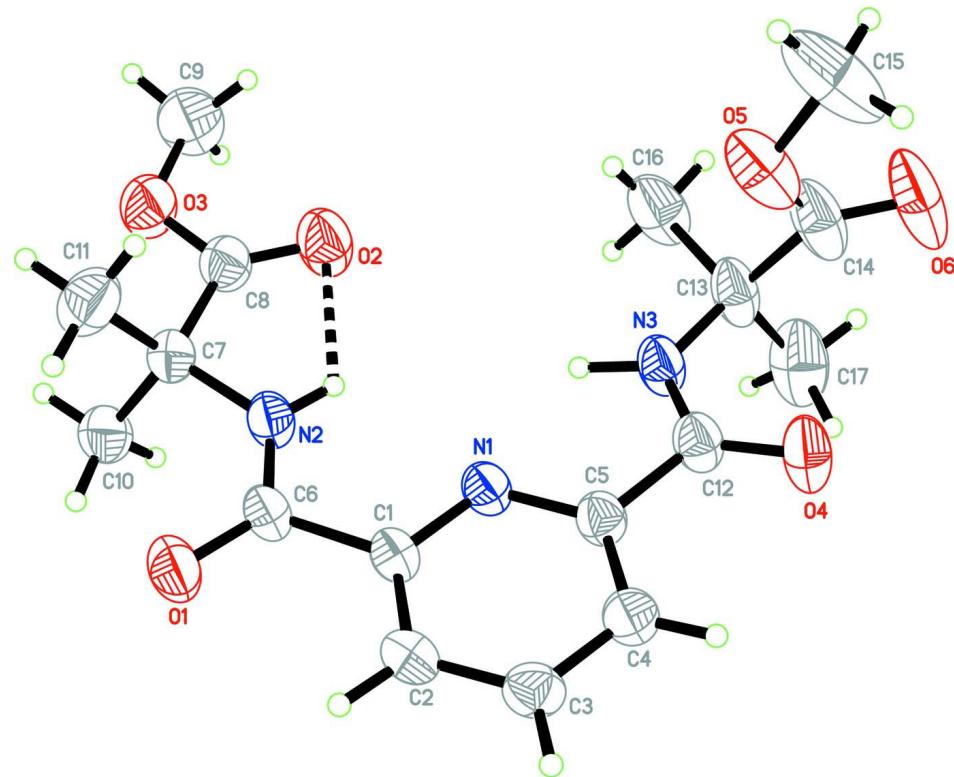
Figure 1

The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms. The intramolecular hydrogen bond is shown as a dashed line.
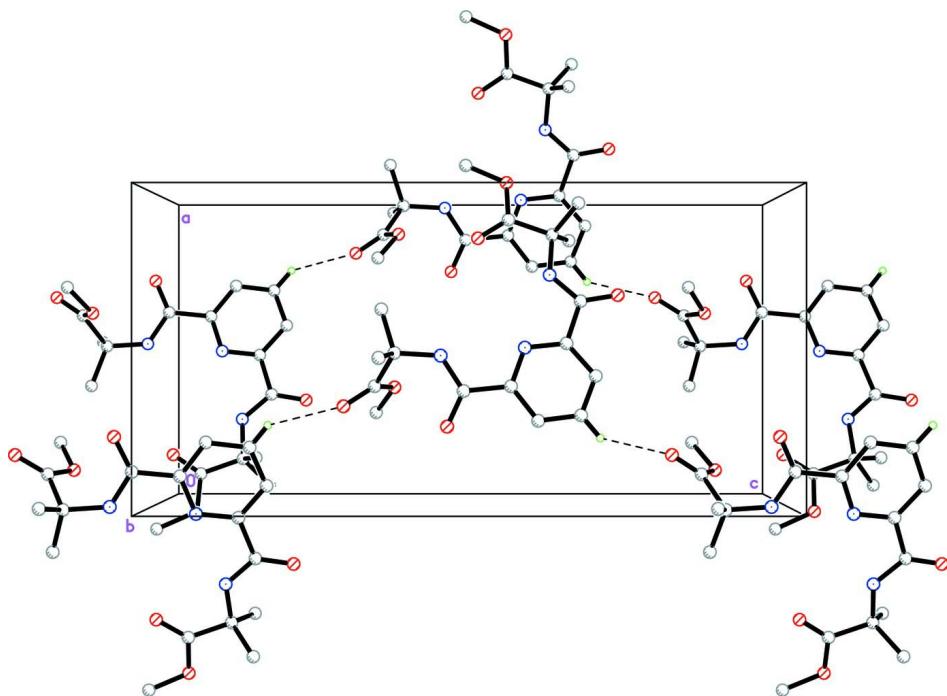
Figure 2

A crystal packing diagram of the title compound, viewed along the *b* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

Methyl 2-({6-[(1-methoxy-2-methyl-1-oxopropan-2- yl)carbamoyl]pyridin-2-yl}formamido)-2-methylpropanoate

Crystal data
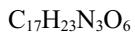
$C_{17}H_{23}N_3O_6$	$F(000) = 776$
$M_r = 365.38$	$D_x = 1.235$ Mg m^{-3}
Orthorhombic, $Pca2_1$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Hall symbol: P 2c -2ac	Cell parameters from 874 reflections
$a = 10.2307\ (10)$ Å	$\theta = 4.8$–$49.5°$
$b = 9.3038\ (11)$ Å	$\mu = 0.79$ mm^{-1}
$c = 20.652\ (2)$ Å	$T = 296$ K
$V = 1965.8\ (4)$ Å^3	Plate, colourless
$Z = 4$	$0.63 \times 0.52 \times 0.09$ mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	7477 measured reflections
	1898 independent reflections
Radiation source: fine-focus sealed tube	1249 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.043$
φ and ω scans	$\theta_{max} = 70.3°$, $\theta_{min} = 6.4°$
Absorption correction: multi-scan	$h = -12 \rightarrow 10$
(*SADABS*; Bruker, 2009)	$k = -10 \rightarrow 11$
$T_{min} = 0.560$, $T_{max} = 0.932$	$l = -24 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from
Least-squares matrix: full	neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H atoms treated by a mixture of independent
$wR(F^2) = 0.133$	and constrained refinement
$S = 0.91$	$w = 1/[\sigma^2(F_o^2) + (0.0914P)^2]$
1898 reflections	where $P = (F_o^2 + 2F_c^2)/3$
250 parameters	$(\Delta/\sigma)_{max} = 0.001$
1 restraint	$\Delta\rho_{max} = 0.19$ e Å^{-3}
Primary atom site location: structure-invariant	$\Delta\rho_{min} = -0.17$ e Å^{-3}
direct methods	Extinction correction: *SHELXTL* (Sheldrick,
Secondary atom site location: difference Fourier	2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
map	Extinction coefficient: 0.0102 (11)

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 > 2sigma(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}
O1	0.6692 (3)	0.7355 (4)	0.72873 (15)	0.1024 (10)
O2	0.8492 (3)	0.6849 (5)	0.51295 (18)	0.1213 (13)
O3	1.0304 (3)	0.5979 (4)	0.55776 (19)	0.1156 (12)
O4	0.2658 (2)	0.9156 (4)	0.46691 (14)	0.1017 (11)
O5	0.3806 (4)	0.6611 (7)	0.3829 (2)	0.1392 (17)
O6	0.3250 (4)	0.8241 (7)	0.3084 (2)	0.170 (2)
N1	0.5055 (3)	0.8326 (3)	0.58446 (14)	0.0676 (8)
N2	0.7327 (3)	0.7306 (4)	0.62369 (18)	0.0745 (8)
H1N2	0.715 (4)	0.744 (4)	0.584 (2)	0.068 (12)*
N3	0.4811 (3)	0.8725 (5)	0.45674 (16)	0.0830 (10)
H1N3	0.554 (5)	0.851 (5)	0.484 (3)	0.102 (14)*
C1	0.5188 (3)	0.8156 (4)	0.64814 (17)	0.0665 (9)
C2	0.4185 (4)	0.8403 (4)	0.69200 (19)	0.0740 (10)
H2A	0.4315	0.8263	0.7361	0.089*
C3	0.2992 (4)	0.8860 (5)	0.66876 (19)	0.0774 (10)
H3A	0.2308	0.9055	0.6971	0.093*
C4	0.2830 (3)	0.9021 (5)	0.60377 (18)	0.0737 (10)
H4A	0.2027	0.9306	0.5870	0.088*
C5	0.3875 (3)	0.8757 (4)	0.5630 (2)	0.0684 (9)
C6	0.6502 (3)	0.7562 (5)	0.67077 (17)	0.0720 (9)
C7	0.8613 (3)	0.6622 (4)	0.6287 (2)	0.0741 (9)
C8	0.9097 (4)	0.6522 (5)	0.5605 (2)	0.0862 (11)
C9	1.0870 (6)	0.5824 (10)	0.4936 (3)	0.147 (3)
H9A	1.1591	0.5165	0.4954	0.220*

H9B	1.1173	0.6742	0.4786	0.220*
H9C	1.0219	0.5462	0.4643	0.220*
C10	0.9549 (4)	0.7569 (6)	0.6675 (3)	0.1005 (15)
H10A	0.9658	0.8474	0.6458	0.151*
H10B	1.0381	0.7099	0.6712	0.151*
H10C	0.9196	0.7731	0.7100	0.151*
C11	0.8503 (6)	0.5137 (6)	0.6576 (3)	0.1151 (17)
H11A	0.7937	0.4559	0.6313	0.173*
H11B	0.8149	0.5205	0.7006	0.173*
H11C	0.9353	0.4703	0.6595	0.173*
C12	0.3733 (3)	0.8903 (5)	0.49148 (19)	0.0774 (11)
C13	0.4893 (4)	0.8851 (7)	0.3870 (2)	0.0988 (17)
C14	0.3863 (4)	0.7913 (10)	0.3552 (2)	0.121 (2)
C15	0.2980 (11)	0.5560 (12)	0.3517 (4)	0.212 (5)
H15A	0.3126	0.4633	0.3709	0.317*
H15B	0.3185	0.5520	0.3064	0.317*
H15C	0.2080	0.5827	0.3571	0.317*
C16	0.6234 (4)	0.8267 (9)	0.3661 (3)	0.135 (3)
H16A	0.6336	0.7301	0.3816	0.203*
H16B	0.6912	0.8862	0.3838	0.203*
H16C	0.6291	0.8273	0.3197	0.203*
C17	0.4747 (6)	1.0409 (9)	0.3669 (3)	0.143 (3)
H17A	0.4022	1.0830	0.3896	0.215*
H17B	0.4594	1.0461	0.3211	0.215*
H17C	0.5533	1.0924	0.3774	0.215*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.101 (2)	0.140 (3)	0.0657 (19)	0.0175 (18)	−0.0122 (14)	0.0065 (18)
O2	0.096 (2)	0.188 (4)	0.080 (2)	0.027 (2)	0.0005 (17)	0.002 (2)
O3	0.0874 (19)	0.157 (3)	0.102 (3)	0.0322 (18)	0.0008 (16)	−0.005 (2)
O4	0.0631 (13)	0.167 (3)	0.0754 (17)	0.0001 (15)	−0.0090 (13)	0.0276 (19)
O5	0.133 (3)	0.200 (5)	0.085 (3)	−0.049 (3)	−0.009 (2)	−0.016 (3)
O6	0.114 (3)	0.318 (7)	0.078 (2)	−0.045 (4)	−0.038 (2)	0.024 (3)
N1	0.0623 (15)	0.085 (2)	0.0558 (18)	−0.0025 (14)	−0.0017 (11)	−0.0001 (14)
N2	0.0652 (15)	0.096 (2)	0.0620 (19)	0.0030 (14)	−0.0075 (14)	0.0038 (18)
N3	0.0638 (16)	0.130 (3)	0.0552 (18)	0.0040 (16)	−0.0019 (13)	0.0054 (17)
C1	0.0708 (19)	0.074 (2)	0.054 (2)	−0.0044 (15)	−0.0051 (14)	0.0036 (17)
C2	0.085 (2)	0.080 (2)	0.057 (2)	−0.0078 (18)	0.0009 (17)	−0.005 (2)
C3	0.071 (2)	0.090 (3)	0.071 (3)	−0.0034 (19)	0.0125 (17)	−0.008 (2)
C4	0.0646 (19)	0.088 (3)	0.068 (2)	−0.0023 (17)	0.0045 (15)	−0.0001 (19)
C5	0.0603 (17)	0.081 (2)	0.064 (2)	−0.0025 (15)	−0.0025 (15)	−0.0004 (18)
C6	0.075 (2)	0.087 (3)	0.054 (2)	−0.0019 (18)	−0.0104 (16)	0.0023 (18)
C7	0.0707 (19)	0.079 (2)	0.072 (2)	0.0061 (17)	−0.0080 (17)	0.001 (2)
C8	0.072 (2)	0.101 (3)	0.086 (3)	0.0066 (19)	−0.005 (2)	−0.004 (3)
C9	0.104 (4)	0.217 (8)	0.118 (4)	0.037 (4)	0.019 (3)	−0.021 (5)
C10	0.078 (2)	0.123 (4)	0.100 (3)	0.012 (2)	−0.020 (2)	−0.019 (3)
C11	0.125 (4)	0.100 (4)	0.121 (4)	0.025 (3)	0.010 (3)	0.021 (3)
C12	0.0661 (19)	0.105 (3)	0.061 (2)	−0.0039 (18)	−0.0013 (16)	0.008 (2)

C13	0.066 (2)	0.174 (5)	0.056 (2)	−0.004 (2)	−0.0016 (15)	0.014 (3)
C14	0.086 (3)	0.222 (7)	0.056 (3)	−0.027 (3)	−0.004 (2)	0.012 (4)
C15	0.227 (10)	0.274 (12)	0.134 (6)	−0.117 (9)	−0.011 (6)	−0.065 (7)
C16	0.076 (3)	0.249 (8)	0.081 (3)	−0.005 (3)	0.010 (2)	−0.032 (4)
C17	0.111 (4)	0.213 (8)	0.106 (4)	−0.015 (4)	0.003 (3)	0.066 (5)

Geometric parameters (Å, º)

O1—C6	1.228 (5)	C7—C8	1.497 (6)
O2—C8	1.200 (6)	C7—C11	1.509 (7)
O3—C8	1.335 (5)	C7—C10	1.528 (6)
O3—C9	1.454 (7)	C9—H9A	0.9600
O4—C12	1.234 (4)	C9—H9B	0.9600
O5—C14	1.341 (9)	C9—H9C	0.9600
O5—C15	1.444 (8)	C10—H10A	0.9600
O6—C14	1.191 (6)	C10—H10B	0.9600
N1—C1	1.332 (5)	C10—H10C	0.9600
N1—C5	1.347 (4)	C11—H11A	0.9600
N2—C6	1.309 (5)	C11—H11B	0.9600
N2—C7	1.466 (5)	C11—H11C	0.9600
N2—H1N2	0.84 (4)	C13—C17	1.516 (9)
N3—C12	1.326 (5)	C13—C14	1.518 (8)
N3—C13	1.447 (6)	C13—C16	1.538 (7)
N3—H1N3	0.95 (5)	C15—H15A	0.9600
C1—C2	1.387 (5)	C15—H15B	0.9600
C1—C6	1.527 (5)	C15—H15C	0.9600
C2—C3	1.379 (6)	C16—H16A	0.9600
C2—H2A	0.9300	C16—H16B	0.9600
C3—C4	1.361 (6)	C16—H16C	0.9600
C3—H3A	0.9300	C17—H17A	0.9600
C4—C5	1.382 (5)	C17—H17B	0.9600
C4—H4A	0.9300	C17—H17C	0.9600
C5—C12	1.491 (6)		
C8—O3—C9	116.4 (4)	C7—C10—H10A	109.5
C14—O5—C15	116.6 (7)	C7—C10—H10B	109.5
C1—N1—C5	116.8 (3)	H10A—C10—H10B	109.5
C6—N2—C7	127.2 (4)	C7—C10—H10C	109.5
C6—N2—H1N2	123 (3)	H10A—C10—H10C	109.5
C7—N2—H1N2	109 (3)	H10B—C10—H10C	109.5
C12—N3—C13	125.2 (3)	C7—C11—H11A	109.5
C12—N3—H1N3	111 (3)	C7—C11—H11B	109.5
C13—N3—H1N3	123 (3)	H11A—C11—H11B	109.5
N1—C1—C2	123.4 (3)	C7—C11—H11C	109.5
N1—C1—C6	115.8 (3)	H11A—C11—H11C	109.5
C2—C1—C6	120.7 (3)	H11B—C11—H11C	109.5
C3—C2—C1	118.6 (4)	O4—C12—N3	122.9 (4)
C3—C2—H2A	120.7	O4—C12—C5	120.8 (3)
C1—C2—H2A	120.7	N3—C12—C5	116.3 (3)
C4—C3—C2	119.0 (4)	N3—C13—C17	110.1 (5)

C4—C3—H3A	120.5	N3—C13—C14	110.1 (4)
C2—C3—H3A	120.5	C17—C13—C14	111.3 (5)
C3—C4—C5	119.1 (4)	N3—C13—C16	107.6 (4)
C3—C4—H4A	120.4	C17—C13—C16	110.4 (5)
C5—C4—H4A	120.4	C14—C13—C16	107.2 (5)
N1—C5—C4	123.1 (4)	O6—C14—O5	123.7 (7)
N1—C5—C12	116.1 (3)	O6—C14—C13	124.6 (8)
C4—C5—C12	120.8 (3)	O5—C14—C13	111.4 (4)
O1—C6—N2	126.4 (4)	O5—C15—H15A	109.5
O1—C6—C1	119.7 (4)	O5—C15—H15B	109.5
N2—C6—C1	114.0 (3)	H15A—C15—H15B	109.5
N2—C7—C8	104.9 (3)	O5—C15—H15C	109.5
N2—C7—C11	111.0 (4)	H15A—C15—H15C	109.5
C8—C7—C11	109.9 (4)	H15B—C15—H15C	109.5
N2—C7—C10	110.5 (3)	C13—C16—H16A	109.5
C8—C7—C10	108.8 (4)	C13—C16—H16B	109.5
C11—C7—C10	111.6 (4)	H16A—C16—H16B	109.5
O2—C8—O3	122.6 (4)	C13—C16—H16C	109.5
O2—C8—C7	125.8 (4)	H16A—C16—H16C	109.5
O3—C8—C7	111.7 (4)	H16B—C16—H16C	109.5
O3—C9—H9A	109.5	C13—C17—H17A	109.5
O3—C9—H9B	109.5	C13—C17—H17B	109.5
H9A—C9—H9B	109.5	H17A—C17—H17B	109.5
O3—C9—H9C	109.5	C13—C17—H17C	109.5
H9A—C9—H9C	109.5	H17A—C17—H17C	109.5
H9B—C9—H9C	109.5	H17B—C17—H17C	109.5
C5—N1—C1—C2	−0.2 (5)	C11—C7—C8—O2	114.7 (6)
C5—N1—C1—C6	175.6 (4)	C10—C7—C8—O2	−122.9 (5)
N1—C1—C2—C3	−0.6 (6)	N2—C7—C8—O3	176.8 (4)
C6—C1—C2—C3	−176.2 (4)	C11—C7—C8—O3	−63.8 (5)
C1—C2—C3—C4	1.5 (6)	C10—C7—C8—O3	58.6 (5)
C2—C3—C4—C5	−1.6 (7)	C13—N3—C12—O4	2.3 (8)
C1—N1—C5—C4	0.1 (6)	C13—N3—C12—C5	−178.6 (4)
C1—N1—C5—C12	−178.4 (4)	N1—C5—C12—O4	173.0 (4)
C3—C4—C5—N1	0.8 (7)	C4—C5—C12—O4	−5.5 (7)
C3—C4—C5—C12	179.2 (4)	N1—C5—C12—N3	−6.1 (6)
C7—N2—C6—O1	4.9 (7)	C4—C5—C12—N3	175.4 (4)
C7—N2—C6—C1	−174.3 (3)	C12—N3—C13—C17	70.9 (6)
N1—C1—C6—O1	−178.9 (4)	C12—N3—C13—C14	−52.2 (7)
C2—C1—C6—O1	−3.0 (6)	C12—N3—C13—C16	−168.7 (5)
N1—C1—C6—N2	0.3 (5)	C15—O5—C14—O6	2.2 (10)
C2—C1—C6—N2	176.3 (4)	C15—O5—C14—C13	−172.4 (6)
C6—N2—C7—C8	176.8 (4)	N3—C13—C14—O6	141.2 (6)
C6—N2—C7—C11	58.1 (6)	C17—C13—C14—O6	18.8 (8)
C6—N2—C7—C10	−66.1 (5)	C16—C13—C14—O6	−102.1 (8)
C9—O3—C8—O2	1.1 (8)	N3—C13—C14—O5	−44.3 (6)
C9—O3—C8—C7	179.6 (5)	C17—C13—C14—O5	−166.7 (5)
N2—C7—C8—O2	−4.7 (6)	C16—C13—C14—O5	72.4 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1*N*2···O2	0.85 (4)	2.08 (4)	2.614 (5)	120 (3)
C3—H3*A*···O6[i]	0.93	2.49	3.204 (6)	134

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