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The amino alcohol $MeN(CH_2CMe_2OH)_2$

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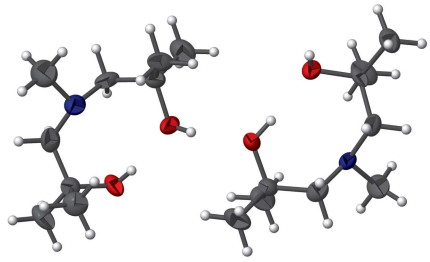
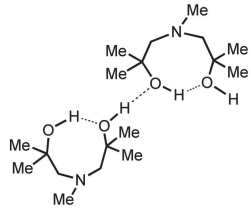
Structural data: full structural data are available from iucrdata.iucr.org

The crystal structure, including a graph-set analysis, of 1-[(2-hydroxy-2-methylpropyl)methylamino]-2-methylpropan-2-ol, $C_9H_{21}NO_2$, is reported. The structure is characterized by unsymmetrical intra- and intermolecular O—H···O hydrogen bridges, giving rise to the formation of an infinite polymer consisting of eight-membered rings arranged in zigzag chains running along the *a* axis.

3D view



Chemical scheme



Structure description

Amino alcohols are an important industrial commodity with widespread applications. Some representatives of these compounds have also characterized by single-crystal X-ray diffraction analysis (Churakov *et al.*, 2009). In the context with our long-standing interest in tin and silicon derivatives of amino alcohols (Berends *et al.*, 2009; Glowacki *et al.*, 2016, 2017; Gock *et al.*, 2013; Iovkova-Berends, Zöller, Bradtmöller *et al.*, 2012; Iovkova-Berends, Berends, Zöller, Schollmeyer *et al.*, 2012; Lutter *et al.*, 2012; Zöller *et al.*, 2011, 2012; Zöller & Jurkschat, 2013), we report here the crystal structure of the title compound (Fig. 1). The latter crystallizes in the orthorhombic space group $Pna2_1$ with eight molecules in the unit cell and two molecules in the asymmetric unit. Each of the crystallographic independent molecules shows an intramolecular O—H···O hydrogen bridge with O11···O17 and O31···O37 distances of 2.621 (4) and 2.715 (4) Å, respectively (Table 1). The two eight-membered rings thus formed are linked by an intermolecular O—H···O hydrogen bridge with an O11···O37 distance of 2.656 (3) Å giving a dimer. The dimers are linked *via* intermolecular O—H···O hydrogen bridges with an O17···O31 distance of 2.712 (3) Å, giving an infinite polymer.

The structure resembles those of $Ph(Me)(H)CN(CH_2CMe_2OH)_2$ (Churakov *et al.*, 2009) and p-$FC_6H_4N(CH_2CMe_2OH)_2$ (Lutter *et al.*, 2012). A graph-set analysis according to Etter and Bernstein (Bernstein *et al.*, 1990, 1995; Bernstein, 1991; Etter, 1990, 1991; Etter *et al.*, 1990) gives the unitary graph set $N_1 = S(8)DS(8)D$.

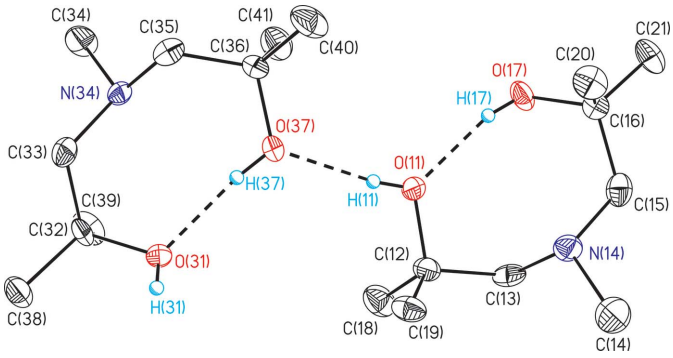


Figure 1
The molecular structure of $MeN(CH_2CMe_2OH)_2$, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms bonded to C atoms have been omitted for clarity. Hydrogen bonds are drawn as dashed lines.

Synthesis and crystallization

The synthesis and the chemical and physical properties of the title compound were published by Hong *et al.* (2008). The latter crystallizes from the melt as colourless column-shaped crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal structure exhibits pseudo symmetry with a percentage fit of 83% for the higher symmetry space group *Pbcn*. However, refinement in the space group *Pbcn* is non-satisfactory.

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

D—H···A	D—H	H···A	D···A	D—H···A
O11—H11···O37	0.76 (2)	1.91 (2)	2.656 (3)	168 (5)
O17—H17···O11	0.80 (2)	1.84 (2)	2.621 (4)	165 (4)
O31—H31···O17^{i}	0.74 (2)	1.99 (2)	2.712 (3)	165 (4)
O37—H37···O31	0.83 (2)	1.89 (2)	2.715 (4)	174 (4)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_9H_{21}NO_2$
M_r	175.27
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	173
a, b, c (Å)	14.152 (2), 9.8983 (16), 15.9939 (19)
V (Å^3)	2240.5 (5)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.40 × 0.19 × 0.06
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Sapphire3
Absorption correction	Multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2006)
T_{min}, T_{max}	0.872, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8013, 4390, 1763
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.045, 0.80
No. of reflections	4390
No. of parameters	239
No. of restraints	5
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.13, −0.15

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2006), *SHELXS* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *enCIFer*(Allen *et al.*, 2004).

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full crystallographic data

IUCrData (2017). **2**, x170799 [https://doi.org/10.1107/S2414314617007994]

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1-[(2-Hydroxy-2-methylpropyl)methylamino]-2-methylpropan-2-ol

Crystal data

$C_9H_{21}NO_2$
M_r = 175.27
Orthorhombic, $Pna2_1$
a = 14.152 (2) Å
b = 9.8983 (16) Å
c = 15.9939 (19) Å
V = 2240.5 (5) Å^3
Z = 8
F(000) = 784
D_x = 1.039 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1703 reflections
θ = 2.4–29.2°
μ = 0.07 mm^{-1}
T = 173 K
Column, colourless
0.40 × 0.19 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Graphite monochromator
Detector resolution: 16.0560 pixels mm^{-1}
ω und ψ scan
Absorption correction: multi-scan (CrysAlis PRO; Oxford Diffraction, 2006)
T_{min} = 0.872, T_{max} = 1.000
8013 measured reflections
4390 independent reflections
1763 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.5°, θ_{min} = 2.4°
h = −14→18
k = −12→6
l = −20→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.045
S = 0.80
4390 reflections
239 parameters
5 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.005P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.036
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack x determined using 585 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).

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. The OH protons were located in the difference Fourier map. Their coordinates were refined using a restraint of O—H = 0.84 (2) Å. The H atoms bonded to C were refined as riding on their parent atom. The U values of all H atoms were set to $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5U_{eq}(C_{methyl},O)$.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O11	0.4659 (2)	0.3733 (3)	0.5278 (2)	0.0561 (9)
H11	0.476 (3)	0.298 (2)	0.522 (3)	0.084*
C12	0.5439 (3)	0.4601 (4)	0.5463 (3)	0.0399 (11)
C13	0.4990 (3)	0.5893 (4)	0.5796 (2)	0.0407 (11)
H13A	0.5490	0.6583	0.5866	0.049*
H13B	0.4537	0.6237	0.5375	0.049*
N14	0.4499 (2)	0.5737 (3)	0.65840 (18)	0.0404 (9)
C14	0.5045 (3)	0.6325 (4)	0.7268 (3)	0.0708 (16)
H14A	0.5671	0.5904	0.7287	0.106*
H14B	0.4716	0.6166	0.7798	0.106*
H14C	0.5113	0.7299	0.7176	0.106*
C15	0.3512 (3)	0.6184 (4)	0.6587 (2)	0.0466 (13)
H15A	0.3439	0.6903	0.6162	0.056*
H15B	0.3373	0.6589	0.7139	0.056*
C16	0.2785 (3)	0.5092 (4)	0.6414 (2)	0.0338 (11)
O17	0.29330 (19)	0.4557 (3)	0.55810 (14)	0.0441 (8)
H17	0.3433 (19)	0.418 (4)	0.554 (2)	0.066*
C18	0.5966 (3)	0.4929 (5)	0.4649 (2)	0.0595 (14)
H18A	0.6225	0.4096	0.4411	0.089*
H18B	0.6482	0.5561	0.4767	0.089*
H18C	0.5526	0.5340	0.4249	0.089*
C19	0.6092 (3)	0.3933 (4)	0.6075 (2)	0.0436 (12)
H19A	0.5750	0.3747	0.6595	0.065*
H19B	0.6627	0.4532	0.6191	0.065*
H19C	0.6324	0.3083	0.5838	0.065*
C20	0.2889 (3)	0.3954 (3)	0.70317 (19)	0.0489 (12)
H20A	0.2439	0.3234	0.6894	0.073*
H20B	0.2761	0.4289	0.7597	0.073*
H20C	0.3534	0.3596	0.7006	0.073*
C21	0.1808 (3)	0.5690 (4)	0.6412 (2)	0.0526 (14)
H21A	0.1346	0.4987	0.6273	0.079*
H21B	0.1774	0.6415	0.5996	0.079*
H21C	0.1665	0.6058	0.6967	0.079*
O31	0.6890 (2)	0.0885 (3)	0.41852 (14)	0.0383 (7)
H31	0.725 (2)	0.081 (4)	0.4514 (19)	0.057*
C32	0.7068 (3)	−0.0168 (4)	0.35925 (19)	0.0330 (11)
C33	0.6370 (3)	−0.1301 (4)	0.3741 (2)	0.0393 (12)

H33A	0.6514	−0.2050	0.3351	0.047*
H33B	0.6454	−0.1645	0.4317	0.047*
N34	0.5380 (2)	−0.0898 (3)	0.36282 (15)	0.0321 (9)
C34	0.4953 (4)	−0.1566 (4)	0.2901 (3)	0.0593 (13)
H34A	0.5305	−0.1322	0.2395	0.089*
H34B	0.4294	−0.1275	0.2843	0.089*
H34C	0.4975	−0.2548	0.2978	0.089*
C35	0.4787 (3)	−0.0994 (4)	0.4377 (2)	0.0409 (12)
H35A	0.5167	−0.1374	0.4841	0.049*
H35B	0.4258	−0.1622	0.4266	0.049*
C36	0.4393 (3)	0.0357 (5)	0.4642 (2)	0.0371 (11)
O37	0.51499 (19)	0.1230 (3)	0.48663 (15)	0.0444 (8)
H37	0.5662 (19)	0.111 (4)	0.463 (2)	0.067*
C38	0.8072 (3)	−0.0694 (4)	0.3662 (2)	0.0495 (13)
H38A	0.8515	0.0066	0.3639	0.074*
H38B	0.8201	−0.1314	0.3198	0.074*
H38C	0.8149	−0.1174	0.4194	0.074*
C39	0.6915 (3)	0.0493 (3)	0.27373 (18)	0.0543 (14)
H39A	0.7316	0.1297	0.2691	0.081*
H39B	0.6251	0.0756	0.2679	0.081*
H39C	0.7081	−0.0150	0.2295	0.081*
C40	0.3803 (3)	0.0181 (5)	0.5426 (2)	0.0577 (13)
H40A	0.4193	−0.0215	0.5869	0.087*
H40B	0.3268	−0.0417	0.5307	0.087*
H40C	0.3567	0.1064	0.5610	0.087*
C41	0.3790 (3)	0.1033 (4)	0.3960 (2)	0.0557 (13)
H41A	0.3523	0.1876	0.4177	0.084*
H41B	0.3277	0.0423	0.3795	0.084*
H41C	0.4187	0.1230	0.3473	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O11	0.0255 (18)	0.039 (2)	0.104 (2)	0.0015 (18)	−0.0051 (17)	−0.029 (2)
C12	0.029 (2)	0.035 (3)	0.055 (2)	−0.002 (2)	0.001 (3)	−0.001 (3)
C13	0.037 (3)	0.031 (3)	0.055 (3)	−0.012 (2)	−0.011 (2)	0.009 (2)
N14	0.034 (2)	0.043 (3)	0.045 (2)	0.002 (2)	−0.0089 (17)	−0.0028 (17)
C14	0.062 (4)	0.095 (4)	0.055 (3)	−0.004 (3)	−0.005 (3)	−0.018 (3)
C15	0.055 (3)	0.035 (3)	0.051 (2)	0.009 (3)	0.004 (2)	−0.001 (2)
C16	0.033 (3)	0.034 (3)	0.034 (2)	0.003 (2)	−0.003 (2)	0.004 (2)
O17	0.0292 (18)	0.068 (2)	0.0355 (16)	0.0103 (16)	−0.0004 (15)	−0.0111 (14)
C18	0.047 (3)	0.086 (4)	0.046 (2)	0.004 (3)	0.002 (3)	0.002 (3)
C19	0.030 (3)	0.043 (3)	0.058 (3)	−0.001 (2)	−0.006 (2)	0.012 (2)
C20	0.055 (3)	0.051 (3)	0.040 (2)	−0.001 (2)	−0.001 (2)	0.012 (2)
C21	0.038 (3)	0.070 (4)	0.050 (2)	0.021 (3)	0.008 (2)	0.008 (2)
O31	0.0303 (18)	0.0394 (17)	0.0452 (16)	0.0008 (15)	−0.0075 (13)	−0.0113 (15)
C32	0.023 (2)	0.046 (3)	0.030 (2)	0.012 (2)	0.003 (2)	−0.002 (2)
C33	0.049 (3)	0.035 (3)	0.034 (2)	−0.001 (2)	0.002 (2)	−0.0092 (19)

N34	0.030 (2)	0.032 (2)	0.034 (2)	−0.0035 (18)	−0.0050 (18)	−0.0084 (16)
C34	0.043 (3)	0.089 (4)	0.046 (2)	0.000 (3)	−0.014 (2)	−0.028 (3)
C35	0.047 (3)	0.038 (3)	0.037 (3)	−0.005 (2)	−0.006 (2)	0.001 (2)
C36	0.029 (3)	0.040 (3)	0.041 (2)	−0.003 (2)	0.006 (2)	−0.003 (2)
O37	0.0283 (19)	0.043 (2)	0.0613 (18)	−0.0015 (17)	0.0105 (14)	−0.0197 (15)
C38	0.035 (3)	0.066 (4)	0.047 (2)	0.013 (3)	−0.004 (2)	−0.013 (2)
C39	0.050 (3)	0.072 (4)	0.041 (2)	0.011 (3)	0.008 (2)	0.023 (2)
C40	0.040 (3)	0.083 (4)	0.050 (2)	−0.007 (3)	0.014 (3)	0.001 (3)
C41	0.044 (3)	0.065 (3)	0.058 (3)	0.013 (3)	−0.006 (2)	0.006 (3)

Geometric parameters (Å, º)

O11—C12	1.430 (5)	O31—C32	1.431 (4)
O11—H11	0.76 (2)	O31—H31	0.74 (2)
C12—C19	1.499 (5)	C32—C33	1.513 (5)
C12—C13	1.525 (5)	C32—C38	1.518 (5)
C12—C18	1.535 (5)	C32—C39	1.532 (4)
C13—N14	1.446 (4)	C33—N34	1.468 (5)
C13—H13A	0.9900	C33—H33A	0.9900
C13—H13B	0.9900	C33—H33B	0.9900
N14—C14	1.459 (4)	N34—C35	1.465 (4)
N14—C15	1.465 (4)	N34—C34	1.468 (4)
C14—H14A	0.9800	C34—H34A	0.9800
C14—H14B	0.9800	C34—H34B	0.9800
C14—H14C	0.9800	C34—H34C	0.9800
C15—C16	1.517 (5)	C35—C36	1.510 (5)
C15—H15A	0.9900	C35—H35A	0.9900
C15—H15B	0.9900	C35—H35B	0.9900
C16—O17	1.449 (4)	C36—O37	1.423 (5)
C16—C20	1.506 (4)	C36—C40	1.516 (5)
C16—C21	1.505 (5)	C36—C41	1.539 (5)
O17—H17	0.80 (2)	O37—H37	0.83 (2)
C18—H18A	0.9800	C38—H38A	0.9800
C18—H18B	0.9800	C38—H38B	0.9800
C18—H18C	0.9800	C38—H38C	0.9800
C19—H19A	0.9800	C39—H39A	0.9800
C19—H19B	0.9800	C39—H39B	0.9800
C19—H19C	0.9800	C39—H39C	0.9800
C20—H20A	0.9800	C40—H40A	0.9800
C20—H20B	0.9800	C40—H40B	0.9800
C20—H20C	0.9800	C40—H40C	0.9800
C21—H21A	0.9800	C41—H41A	0.9800
C21—H21B	0.9800	C41—H41B	0.9800
C21—H21C	0.9800	C41—H41C	0.9800
C12—O11—H11	118 (4)	C32—O31—H31	106 (3)
O11—C12—C19	110.2 (4)	O31—C32—C33	108.7 (3)
O11—C12—C13	104.8 (3)	O31—C32—C38	111.4 (3)

C19—C12—C13	113.5 (4)	C33—C32—C38	110.2 (4)
O11—C12—C18	109.0 (4)	O31—C32—C39	104.8 (3)
C19—C12—C18	110.4 (3)	C33—C32—C39	111.4 (3)
C13—C12—C18	108.8 (3)	C38—C32—C39	110.1 (3)
N14—C13—C12	114.5 (3)	N34—C33—C32	113.7 (3)
N14—C13—H13A	108.6	N34—C33—H33A	108.8
C12—C13—H13A	108.6	C32—C33—H33A	108.8
N14—C13—H13B	108.6	N34—C33—H33B	108.8
C12—C13—H13B	108.6	C32—C33—H33B	108.8
H13A—C13—H13B	107.6	H33A—C33—H33B	107.7
C13—N14—C14	110.8 (4)	C33—N34—C35	115.4 (3)
C13—N14—C15	115.3 (3)	C33—N34—C34	111.6 (3)
C14—N14—C15	112.4 (3)	C35—N34—C34	112.5 (3)
N14—C14—H14A	109.5	N34—C34—H34A	109.5
N14—C14—H14B	109.5	N34—C34—H34B	109.5
H14A—C14—H14B	109.5	H34A—C34—H34B	109.5
N14—C14—H14C	109.5	N34—C34—H34C	109.5
H14A—C14—H14C	109.5	H34A—C34—H34C	109.5
H14B—C14—H14C	109.5	H34B—C34—H34C	109.5
N14—C15—C16	115.5 (4)	N34—C35—C36	112.6 (3)
N14—C15—H15A	108.4	N34—C35—H35A	109.1
C16—C15—H15A	108.4	C36—C35—H35A	109.1
N14—C15—H15B	108.4	N34—C35—H35B	109.1
C16—C15—H15B	108.4	C36—C35—H35B	109.1
H15A—C15—H15B	107.5	H35A—C35—H35B	107.8
O17—C16—C20	108.4 (3)	O37—C36—C35	109.3 (3)
O17—C16—C21	105.9 (3)	O37—C36—C40	106.0 (3)
C20—C16—C21	112.6 (3)	C35—C36—C40	109.6 (4)
O17—C16—C15	109.3 (3)	O37—C36—C41	109.4 (3)
C20—C16—C15	110.3 (3)	C35—C36—C41	113.0 (3)
C21—C16—C15	110.1 (4)	C40—C36—C41	109.4 (4)
C16—O17—H17	112 (3)	C36—O37—H37	117 (3)
C12—C18—H18A	109.5	C32—C38—H38A	109.5
C12—C18—H18B	109.5	C32—C38—H38B	109.5
H18A—C18—H18B	109.5	H38A—C38—H38B	109.5
C12—C18—H18C	109.5	C32—C38—H38C	109.5
H18A—C18—H18C	109.5	H38A—C38—H38C	109.5
H18B—C18—H18C	109.5	H38B—C38—H38C	109.5
C12—C19—H19A	109.5	C32—C39—H39A	109.5
C12—C19—H19B	109.5	C32—C39—H39B	109.5
H19A—C19—H19B	109.5	H39A—C39—H39B	109.5
C12—C19—H19C	109.5	C32—C39—H39C	109.5
H19A—C19—H19C	109.5	H39A—C39—H39C	109.5
H19B—C19—H19C	109.5	H39B—C39—H39C	109.5
C16—C20—H20A	109.5	C36—C40—H40A	109.5
C16—C20—H20B	109.5	C36—C40—H40B	109.5
H20A—C20—H20B	109.5	H40A—C40—H40B	109.5
C16—C20—H20C	109.5	C36—C40—H40C	109.5

H20A—C20—H20C	109.5	H40A—C40—H40C	109.5
H20B—C20—H20C	109.5	H40B—C40—H40C	109.5
C16—C21—H21A	109.5	C36—C41—H41A	109.5
C16—C21—H21B	109.5	C36—C41—H41B	109.5
H21A—C21—H21B	109.5	H41A—C41—H41B	109.5
C16—C21—H21C	109.5	C36—C41—H41C	109.5
H21A—C21—H21C	109.5	H41A—C41—H41C	109.5
H21B—C21—H21C	109.5	H41B—C41—H41C	109.5
O11—C12—C13—N14	65.9 (4)	O31—C32—C33—N34	61.5 (4)
C19—C12—C13—N14	−54.4 (5)	C38—C32—C33—N34	−176.0 (3)
C18—C12—C13—N14	−177.7 (3)	C39—C32—C33—N34	−53.5 (4)
C12—C13—N14—C14	105.6 (4)	C32—C33—N34—C35	−117.1 (4)
C12—C13—N14—C15	−125.2 (4)	C32—C33—N34—C34	112.8 (4)
C13—N14—C15—C16	94.1 (4)	C33—N34—C35—C36	118.2 (4)
C14—N14—C15—C16	−137.5 (3)	C34—N34—C35—C36	−112.2 (4)
N14—C15—C16—O17	−62.5 (4)	N34—C35—C36—O37	−63.3 (4)
N14—C15—C16—C20	56.6 (4)	N34—C35—C36—C40	−179.0 (3)
N14—C15—C16—C21	−178.5 (3)	N34—C35—C36—C41	58.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H11···O37	0.76 (2)	1.91 (2)	2.656 (3)	168 (5)
O17—H17···O11	0.80 (2)	1.84 (2)	2.621 (4)	165 (4)
O31—H31···O17^{i}	0.74 (2)	1.99 (2)	2.712 (3)	165 (4)
O37—H37···O31	0.83 (2)	1.89 (2)	2.715 (4)	174 (4)

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