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tert-Butyl *N*-[(*S*)-3-isopropyl-2-oxo-oxetan-3-yl]carbamate

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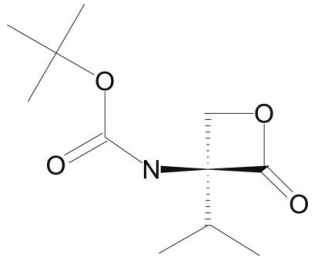
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.104; data-to-parameter ratio = 8.7.

The structure of the title compound, $C_{11}H_{19}NO_4$, contains two crystallographically independent molecules in the asymmetric unit. Both adopt the same conformation and they form pseudosymmetric $R_2^2(8)$ dimers *via* two N—H···O hydrogen bonds. The dimers are linked by weak C—H···O interactions and are stacked in columns along the *a* axis.

Related literature

For related literature, see: Etter *et al.* (1990); Lall *et al.* (2002); Lowe & Vederas (1995); Olma & Kudaj (2005); Sieroń *et al.* (2008); Smith & Goodman (2003).



Experimental

Crystal data

$C_{11}H_{19}NO_4$
M_r = 229.27
Monoclinic, $P2_1$
a = 6.0475 (2) Å
b = 20.8957 (6) Å
c = 10.2928 (3) Å
β = 94.675 (3)°
V = 1296.34 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.4 × 0.3 × 0.3 mm

Data collection

Kuma KM-4-CCD diffractometer
Absorption correction: none
19342 measured reflections
2615 independent reflections
2118 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.103
S = 1.02
2615 reflections
299 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8···O29	0.86	2.09	2.939 (2)	169
N28—H28···O9	0.86	2.08	2.924 (3)	168
C6—H6*C*···O29	0.96	2.54	3.434 (4)	154
C27—H27*C*···O9	0.96	2.57	3.442 (4)	151

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GD2021).

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supplementary materials

Acta Cryst. (2008). E**64**, o550 [**doi:10.1107/S1600536808003279**]

tert-Butyl *N*-[(*S*)-3-isopropyl-2-oxooxetan-3-yl]carbamate

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Comment

Over the last 20 years, much attention has been focused on β-lactones, because their occurrence in many natural biologically active compounds (Lowe & Vederas, 1995). *N*-Cbz-serine and threonine β-lactones have been found as a new class of hepatitis A virus 3 C cysteine proteinase inhibitors (Lall *et al.*, 2002).

The crystal structure of the title compound, (I), is related to this area of interest. The title compound - useful and versatile intermediate in the synthesis of β-substituted α-alkyl alanines was prepared according to standard procedure (Olma & Kudaj, 2005).

The asymmetric unit in the crystal structure of (I) contains two molecules. Both molecules in (I) are practically identical. The pairs of the molecules are connected into the same motif as observed in the structures of other *N*-protected-α-amino-β-lactones (Sieroń, *et al.*, 2008; Smith & Goodman, 2003). Therefore the molecules are connected in pesudocentrosymmetric dimers *via* N–H···O hydrogen bonds, forming eight-membered rings described by the $R_2^2(8)$ graph-set motif (Etter *et al.*, 1990) (Fig. 1). In the crystal of (I) dimers are stacked down the α-axis in columns.

Experimental

The title compound was synthesized by treating complex of triphenylphosphine (525 mg, 2 mmol) and diethyldiazadicarboxylate in dry tetrahydrofurane with solution of Boc-(*S*)-*iso*-propylserine (*N*-Boc-(*S*)-hydroxymethylvaline) in dry THF (670 mg, 2 mmol) at 0°C. After stirring 1 h at 0°C and then 16 h at room temperature, THF was removed *in vacuo* and the crude product was purified by flash chromatography on silica gel 60 (230–400 mesh) using ethyl acetate-*n*-hexane (1:1) aseluent·The *N*-Boc-(*S*)-α-benzylserine lactone was obtained in 92% yield. White crystals of *N*-Boc-(*S*)-α-*iso*-propylserine lactone suitable for X-ray investigation were grown from chloroform, m.p. 403–404 K.

Refinement

In the absence of significant anomalous scattering effects, Friedel pairs were merged. The absolute configuration was assigned consistent with the starting material. All H atoms were included in calculated positions and treated as riding, C–H = 0.96–0.98 and N–H = 0.86 Å with U_{iso}(H) = 1.2 or 1.5U_{eq}(C) and 1.2U_{eq}(N).

Figures

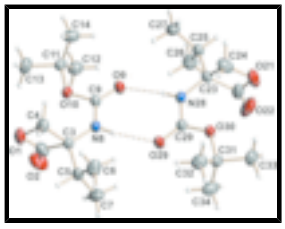


Fig. 1. The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Dotted lines indicate hydrogen bonds.

tert-Butyl *N*-[(*S*)-3-isopropyl-2-oxooxetan-3-yl]carbamate

Crystal data

$C_{11}H_{19}NO_4$	F_{000} = 496
M_r = 229.27	D_x = 1.175 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 11196 reflections
a = 6.0475 (2) Å	θ = 1.9–28.0º
b = 20.8957 (6) Å	μ = 0.09 mm^{-1}
c = 10.2928 (3) Å	T = 298 K
β = 94.675 (3)º	Rectangular plate, colourless
V = 1296.34 (7) Å^3	0.4 × 0.3 × 0.3 mm
Z = 4	

Data collection

Kuma KM-4-CCD diffractometer	2118 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
Detector resolution: 8.2356 pixels mm^{-1}	θ_{max} = 26.0º
T = 298 K	θ_{min} = 2.2º
ω scans	h = −7→7
Absorption correction: none	k = −23→25
19342 measured reflections	l = −12→12
2615 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.103	$w = 1/[\sigma^2(F_o^2) + (0.0757P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$

2615 reflections	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
299 parameters	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
1 restraint	Extinction correction: SHELXTL (Bruker, 2000), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.023 (5)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating –*R*-factor-obs *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	0.6494 (4)	0.23045 (10)	0.63037 (19)	0.0829 (8)
O2	0.8994 (4)	0.25263 (14)	0.4835 (3)	0.1062 (10)
O9	0.2398 (3)	0.27971 (8)	0.20705 (16)	0.0622 (6)
O10	0.4114 (3)	0.21360 (7)	0.35786 (15)	0.0564 (5)
N8	0.4182 (3)	0.31805 (8)	0.39179 (17)	0.0497 (6)
C2	0.7305 (5)	0.26212 (14)	0.5292 (3)	0.0688 (10)
C3	0.5404 (4)	0.31069 (10)	0.5160 (2)	0.0468 (6)
C4	0.4449 (5)	0.26711 (14)	0.6194 (2)	0.0664 (9)
C5	0.6185 (5)	0.37608 (11)	0.5715 (2)	0.0595 (8)
C6	0.4225 (6)	0.41648 (14)	0.6078 (3)	0.0806 (13)
C7	0.7639 (6)	0.41090 (18)	0.4834 (3)	0.0893 (11)
C9	0.3479 (4)	0.27053 (10)	0.3106 (2)	0.0489 (7)
C11	0.3517 (4)	0.15329 (10)	0.2879 (2)	0.0535 (7)
C12	0.4526 (5)	0.15184 (14)	0.1587 (3)	0.0698 (10)
C13	0.4626 (7)	0.10416 (14)	0.3800 (4)	0.0905 (13)
C14	0.1059 (5)	0.14520 (14)	0.2731 (3)	0.0751 (10)
O21	−0.3083 (4)	0.48529 (11)	−0.0728 (2)	0.1029 (10)
O22	0.0293 (6)	0.47727 (12)	−0.1507 (2)	0.1157 (12)
O29	0.2623 (3)	0.44185 (7)	0.28415 (17)	0.0670 (6)
O30	0.0350 (3)	0.50520 (7)	0.15453 (15)	0.0591 (5)
N28	0.0285 (3)	0.40040 (9)	0.12378 (16)	0.0503 (6)
C22	−0.1048 (6)	0.45988 (14)	−0.0824 (3)	0.0744 (10)
C23	−0.1359 (4)	0.40626 (11)	0.01507 (19)	0.0490 (7)
C24	−0.3549 (5)	0.44115 (16)	0.0314 (3)	0.0809 (11)
C25	−0.1695 (4)	0.34178 (12)	−0.0555 (2)	0.0544 (7)
C26	0.0390 (6)	0.31841 (15)	−0.1124 (3)	0.0732 (10)

C27	−0.2654 (5)	0.29098 (14)	0.0287 (3)	0.0730 (10)
C29	0.1192 (4)	0.44917 (10)	0.1946 (2)	0.0497 (7)
C31	0.1104 (4)	0.56660 (10)	0.2160 (2)	0.0541 (7)
C32	0.0453 (6)	0.56815 (15)	0.3535 (3)	0.0784 (10)
C33	−0.0211 (6)	0.61481 (14)	0.1317 (3)	0.0854 (11)
C34	0.3547 (5)	0.57527 (15)	0.2071 (3)	0.0800 (10)
H4A	0.41570	0.28940	0.69890	0.0800*
H4B	0.31650	0.24260	0.58610	0.0800*
H5	0.70970	0.36750	0.65270	0.0710*
H6A	0.47620	0.45300	0.65740	0.1210*
H6B	0.32920	0.39130	0.65890	0.1210*
H6C	0.33860	0.43060	0.52980	0.1210*
H7A	0.67700	0.42410	0.40580	0.1340*
H7B	0.88080	0.38300	0.46050	0.1340*
H7C	0.82700	0.44790	0.52760	0.1340*
H8	0.38680	0.35650	0.36680	0.0600*
H12A	0.38010	0.18290	0.10110	0.1050*
H12B	0.43410	0.11000	0.12090	0.1050*
H12C	0.60780	0.16170	0.17180	0.1050*
H13A	0.61900	0.11260	0.39140	0.1360*
H13B	0.43840	0.06210	0.34400	0.1360*
H13C	0.40050	0.10660	0.46270	0.1360*
H14A	0.04660	0.15200	0.35580	0.1130*
H14B	0.07030	0.10270	0.24290	0.1130*
H14C	0.04250	0.17570	0.21110	0.1130*
H24A	−0.48530	0.41480	0.01090	0.0970*
H24B	−0.36060	0.46160	0.11560	0.0970*
H25	−0.27950	0.34910	−0.12930	0.0650*
H26A	0.14850	0.30770	−0.04300	0.1100*
H26B	0.09550	0.35150	−0.16530	0.1100*
H26C	0.00510	0.28120	−0.16500	0.1100*
H27A	−0.29710	0.25310	−0.02230	0.1100*
H27B	−0.39980	0.30660	0.06100	0.1100*
H27C	−0.16020	0.28100	0.10070	0.1100*
H28	0.07240	0.36240	0.14520	0.0600*
H32A	−0.11110	0.56040	0.35370	0.1180*
H32B	0.08010	0.60930	0.39100	0.1180*
H32C	0.12530	0.53560	0.40370	0.1180*
H33A	0.01500	0.61040	0.04310	0.1280*
H33B	0.01550	0.65730	0.16200	0.1280*
H33C	−0.17690	0.60740	0.13650	0.1280*
H34A	0.43440	0.54430	0.26170	0.1200*
H34B	0.39720	0.61760	0.23550	0.1200*
H34C	0.38910	0.56940	0.11850	0.1200*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1	0.1125 (17)	0.0604 (12)	0.0703 (11)	0.0111 (11)	−0.0261 (11)	0.0139 (9)
O2	0.0701 (14)	0.121 (2)	0.1255 (19)	0.0289 (13)	−0.0045 (13)	−0.0300 (16)
O9	0.0816 (12)	0.0452 (9)	0.0549 (9)	0.0060 (8)	−0.0242 (8)	−0.0014 (7)
O10	0.0752 (11)	0.0329 (8)	0.0572 (9)	0.0017 (7)	−0.0190 (7)	−0.0017 (6)
N8	0.0650 (11)	0.0329 (9)	0.0479 (9)	0.0014 (8)	−0.0148 (8)	0.0006 (7)
C2	0.0660 (18)	0.0677 (17)	0.0690 (16)	0.0119 (13)	−0.0178 (13)	−0.0129 (13)
C3	0.0549 (12)	0.0401 (11)	0.0437 (10)	0.0011 (9)	−0.0062 (9)	−0.0013 (8)
C4	0.0836 (18)	0.0597 (16)	0.0548 (13)	−0.0038 (14)	−0.0004 (12)	0.0062 (11)
C5	0.0801 (17)	0.0483 (13)	0.0465 (12)	−0.0082 (12)	−0.0174 (11)	−0.0019 (10)
C6	0.120 (3)	0.0534 (16)	0.0676 (16)	0.0097 (16)	0.0025 (16)	−0.0139 (12)
C7	0.092 (2)	0.084 (2)	0.0889 (19)	−0.0388 (19)	−0.0102 (17)	0.0089 (17)
C9	0.0569 (12)	0.0393 (11)	0.0480 (11)	0.0018 (10)	−0.0107 (9)	0.0003 (9)
C11	0.0625 (14)	0.0343 (11)	0.0623 (13)	−0.0004 (10)	−0.0025 (11)	−0.0064 (9)
C12	0.0778 (17)	0.0534 (15)	0.0787 (18)	−0.0049 (13)	0.0103 (13)	−0.0123 (12)
C13	0.126 (3)	0.0419 (15)	0.099 (2)	0.0051 (16)	−0.0194 (19)	0.0095 (13)
C14	0.0700 (17)	0.0581 (17)	0.097 (2)	−0.0114 (13)	0.0063 (14)	−0.0184 (14)
O21	0.124 (2)	0.0657 (13)	0.1089 (16)	0.0282 (13)	−0.0526 (14)	0.0013 (12)
O22	0.191 (3)	0.0772 (16)	0.0807 (14)	−0.0227 (18)	0.0218 (16)	0.0257 (13)
O29	0.0875 (12)	0.0407 (9)	0.0661 (10)	0.0031 (8)	−0.0337 (9)	−0.0037 (7)
O30	0.0761 (11)	0.0358 (8)	0.0608 (9)	0.0037 (7)	−0.0226 (8)	−0.0020 (7)
N28	0.0638 (11)	0.0355 (9)	0.0490 (9)	0.0023 (8)	−0.0119 (8)	−0.0014 (8)
C22	0.110 (2)	0.0510 (15)	0.0580 (15)	−0.0025 (16)	−0.0194 (15)	0.0069 (11)
C23	0.0553 (12)	0.0462 (12)	0.0433 (10)	0.0034 (10)	−0.0088 (9)	−0.0020 (9)
C24	0.0643 (16)	0.079 (2)	0.096 (2)	0.0137 (14)	−0.0133 (14)	−0.0235 (16)
C25	0.0652 (14)	0.0490 (12)	0.0464 (11)	−0.0050 (11)	−0.0111 (10)	−0.0019 (10)
C26	0.093 (2)	0.0652 (16)	0.0618 (15)	0.0043 (14)	0.0082 (14)	−0.0139 (12)
C27	0.0766 (18)	0.0601 (16)	0.0800 (17)	−0.0185 (13)	−0.0084 (14)	0.0069 (13)
C29	0.0621 (13)	0.0382 (11)	0.0470 (11)	0.0006 (10)	−0.0069 (10)	−0.0006 (9)
C31	0.0646 (14)	0.0326 (11)	0.0634 (13)	0.0001 (10)	−0.0048 (11)	−0.0014 (9)
C32	0.097 (2)	0.0627 (17)	0.0760 (17)	−0.0035 (16)	0.0099 (15)	−0.0136 (14)
C33	0.108 (2)	0.0432 (14)	0.101 (2)	0.0107 (15)	−0.0159 (18)	0.0070 (14)
C34	0.0734 (19)	0.0540 (15)	0.114 (2)	−0.0037 (14)	0.0167 (16)	−0.0104 (15)

Geometric parameters (Å, °)

O1—C2	1.359 (4)	C12—H12C	0.96
O1—C4	1.451 (4)	C12—H12B	0.96
O2—C2	1.176 (4)	C12—H12A	0.96
O9—C9	1.219 (3)	C13—H13C	0.96
O10—C9	1.330 (3)	C13—H13A	0.96
O10—C11	1.481 (3)	C13—H13B	0.96
O21—C24	1.459 (4)	C14—H14B	0.96
O21—C22	1.351 (4)	C14—H14A	0.96
O22—C22	1.173 (5)	C14—H14C	0.96
O29—C29	1.221 (3)	C22—C23	1.526 (4)
O30—C31	1.486 (3)	C23—C25	1.536 (3)
O30—C29	1.329 (3)	C23—C24	1.533 (4)
N8—C3	1.432 (3)	C25—C26	1.514 (4)
N8—C9	1.344 (3)	C25—C27	1.515 (4)

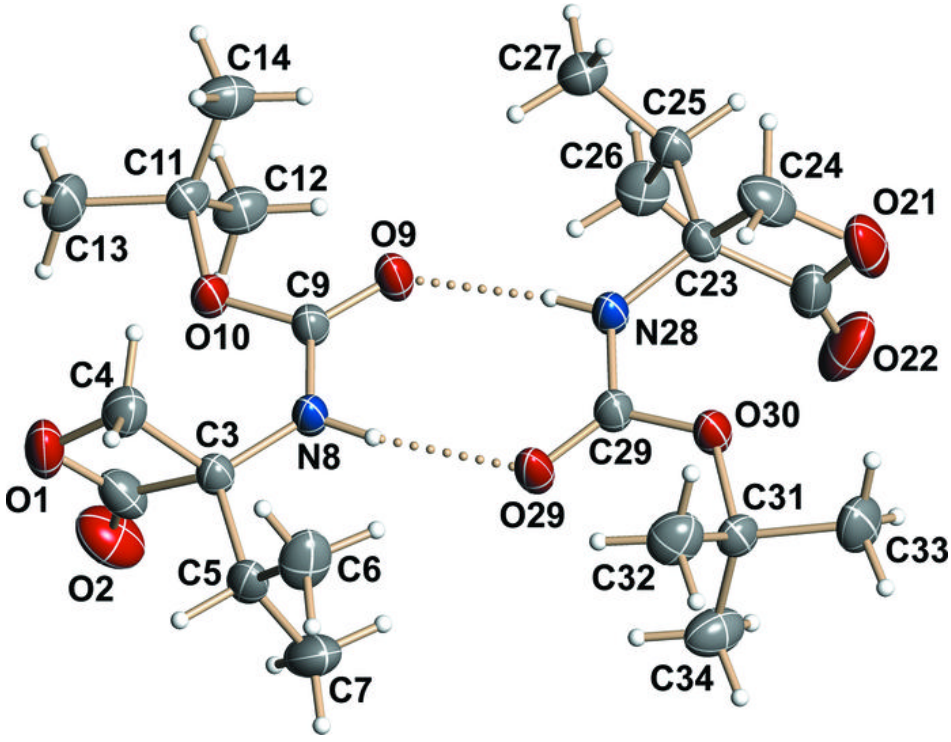
N8—H8	0.86	C31—C33	1.513 (4)
N28—C23	1.440 (3)	C31—C34	1.499 (4)
N28—C29	1.344 (3)	C31—C32	1.500 (4)
N28—H28	0.86	C24—H24A	0.97
C2—C3	1.531 (4)	C24—H24B	0.97
C3—C5	1.540 (3)	C25—H25	0.98
C3—C4	1.548 (3)	C26—H26A	0.96
C5—C7	1.502 (4)	C26—H26B	0.96
C5—C6	1.526 (4)	C26—H26C	0.96
C11—C14	1.492 (4)	C27—H27A	0.96
C11—C12	1.508 (4)	C27—H27B	0.96
C11—C13	1.516 (4)	C27—H27C	0.96
C4—H4A	0.97	C32—H32A	0.96
C4—H4B	0.97	C32—H32B	0.96
C5—H5	0.98	C32—H32C	0.96
C6—H6B	0.96	C33—H33A	0.96
C6—H6C	0.96	C33—H33B	0.96
C6—H6A	0.96	C33—H33C	0.96
C7—H7B	0.96	C34—H34A	0.96
C7—H7C	0.96	C34—H34B	0.96
C7—H7A	0.96	C34—H34C	0.96
C2—O1—C4	92.4 (2)	H14A—C14—H14B	109
C9—O10—C11	122.10 (17)	H14A—C14—H14C	109
C22—O21—C24	92.1 (2)	H14B—C14—H14C	109
C29—O30—C31	122.15 (17)	C11—C14—H14A	109
C3—N8—C9	126.14 (17)	C11—C14—H14B	109
C9—N8—H8	117	O22—C22—C23	138.6 (3)
C3—N8—H8	117	O21—C22—O22	126.9 (3)
C23—N28—C29	125.62 (19)	O21—C22—C23	94.5 (2)
C29—N28—H28	117	N28—C23—C22	117.3 (2)
C23—N28—H28	117	C22—C23—C24	82.9 (2)
O1—C2—C3	94.3 (2)	N28—C23—C24	120.21 (19)
O1—C2—O2	127.2 (3)	N28—C23—C25	110.43 (18)
O2—C2—C3	138.3 (3)	C24—C23—C25	112.8 (2)
C2—C3—C4	82.45 (19)	C22—C23—C25	110.60 (18)
N8—C3—C5	110.87 (17)	O21—C24—C23	90.0 (2)
C2—C3—C5	110.5 (2)	C23—C25—C27	112.71 (19)
N8—C3—C4	118.9 (2)	C23—C25—C26	112.6 (2)
N8—C3—C2	118.66 (19)	C26—C25—C27	111.4 (2)
C4—C3—C5	112.78 (18)	O29—C29—N28	123.2 (2)
O1—C4—C3	90.0 (2)	O29—C29—O30	125.1 (2)
C3—C5—C6	111.1 (2)	O30—C29—N28	111.76 (19)
C6—C5—C7	112.6 (2)	O30—C31—C33	101.66 (19)
C3—C5—C7	112.5 (2)	O30—C31—C34	110.4 (2)
O9—C9—O10	125.4 (2)	C32—C31—C34	113.0 (2)
O9—C9—N8	123.2 (2)	C33—C31—C34	111.1 (2)
O10—C9—N8	111.47 (18)	C32—C31—C33	111.2 (2)
C12—C11—C14	112.3 (2)	O30—C31—C32	108.99 (19)
C13—C11—C14	111.9 (2)	O21—C24—H24A	114

C12—C11—C13	110.3 (2)	O21—C24—H24B	114
O10—C11—C14	110.3 (2)	C23—C24—H24A	114
O10—C11—C12	110.22 (19)	C23—C24—H24B	114
O10—C11—C13	101.20 (19)	H24A—C24—H24B	111
C3—C4—H4B	114	C23—C25—H25	107
C3—C4—H4A	114	C26—C25—H25	107
H4A—C4—H4B	111	C27—C25—H25	107
O1—C4—H4B	114	C25—C26—H26A	109
O1—C4—H4A	114	C25—C26—H26B	109
C6—C5—H5	107	C25—C26—H26C	109
C3—C5—H5	107	H26A—C26—H26B	110
C7—C5—H5	107	H26A—C26—H26C	109
H6A—C6—H6C	109	H26B—C26—H26C	109
C5—C6—H6C	109	C25—C27—H27A	109
H6A—C6—H6B	109	C25—C27—H27B	110
H6B—C6—H6C	109	C25—C27—H27C	109
C5—C6—H6A	110	H27A—C27—H27B	109
C5—C6—H6B	110	H27A—C27—H27C	109
C5—C7—H7A	110	H27B—C27—H27C	109
C5—C7—H7C	109	C31—C32—H32A	109
C5—C7—H7B	109	C31—C32—H32B	109
H7B—C7—H7C	109	C31—C32—H32C	109
H7A—C7—H7C	109	H32A—C32—H32B	110
H7A—C7—H7B	110	H32A—C32—H32C	109
C11—C12—H12B	109	H32B—C32—H32C	110
C11—C12—H12C	109	C31—C33—H33A	109
H12B—C12—H12C	109	C31—C33—H33B	109
H12A—C12—H12B	109	C31—C33—H33C	110
C11—C12—H12A	109	H33A—C33—H33B	109
H12A—C12—H12C	109	H33A—C33—H33C	109
C11—C13—H13C	109	H33B—C33—H33C	109
H13A—C13—H13B	109	C31—C34—H34A	109
C11—C13—H13B	109	C31—C34—H34B	109
C11—C13—H13A	109	C31—C34—H34C	109
H13B—C13—H13C	109	H34A—C34—H34B	109
H13A—C13—H13C	110	H34A—C34—H34C	109
C11—C14—H14C	109	H34B—C34—H34C	109

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N8—H8···O29	0.86	2.09	2.939 (2)	169
N28—H28···O9	0.86	2.08	2.924 (3)	168
C6—H6C···O29	0.96	2.54	3.434 (4)	154
C27—H27C···O9	0.96	2.57	3.442 (4)	151

Fig. 1


C14
C11
C12
C13
O9
C9
O10
C4
C3
N8
O1
O2
C5
C6
C7
C27
C25
C26
C24
O21
C23
N28
O22
O30
C29
O29
C31
C33
C32
C34