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Benzyl 2-{[2-(*tert*-butoxycarbonylamino)-4-methylpentanoyl]methylamino}-4-methylpentanoate

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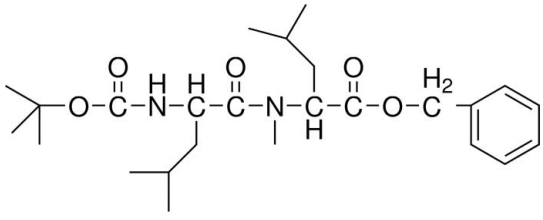
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.099; data-to-parameter ratio = 11.0.

The title compound, $C_{25}H_{40}N_2O_5$, was synthesized in 55.9% yield by condensation of *N*-methyl-L-leucine benzyl ester toluene sulfonic acid with *tert*-butoxycarbonyl-L-leucine at 273 K and its crystal structure determined. The dipeptide derivative conjugates through the amide linkage and includes two protecting groups, a *tert*-butyloxycarbonyl group at the C-tip and a benzyl group at the N-tip.

Related literature

For related literature, see: Schmidt & Potzolli (1987); McKeever & Pattenden (2003).



Experimental

Crystal data

$C_{25}H_{40}N_2O_5$
M_r = 448.59
Orthorhombic, $P2_12_12_1$
a = 9.9400 (12) Å
b = 14.9395 (18) Å
c = 17.876 (2) Å
V = 2654.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
0.50 × 0.40 × 0.20 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.96, T_{max} = 0.99
13652 measured reflections
3277 independent reflections
2732 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.099
S = 1.04
3277 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2061).

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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Benzyl 2-{[2-(*tert*-butoxycarbonylamino)-4-methylpentanoyl]methylamino}-4-methylpentanoate

X.-J. Liao, W.-J. Xu, S.-H. Xu and F.-F. Dong

Comment

Amino acid derivatives are used generally for the synthesis of polypeptides. The title compound, (I), is a product of the reaction of two *L*-Leucine derivatives. It is a precursor for dipeptides, an intermediate product in the synthesis of polypeptides. We report here its crystal structure. The bond lengths and angles are unexceptional and are in good agreement with the corresponding values in *L*-Valine, *N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-*L*-leucyl]-*N*-methyl-phenylmethyl ester (Schmidt *et al.*,1987)

Experimental

N-Methyl-*L*-Leucine benzyl ester Toluene Sulfonic acid (0.82 g, 2 mmol) and diisopropylethylamine (1.3 ml, 7.2 mmol) were added to dichloromethane (5 ml) at room temperature under an atmosphere of nitrogen, On dissolution, the mixture was cooled to 273 K, then 1-hydroxybenzotriazole (0.30 g, 2.2 mmol) and *tert*-Butoxycarbonyl-L– Leucine (0.46 g, 2 mmol) were added successively. After 15 minutes, *N*,*N*'-dicyclohexylcarbodiimide (0.45 g, 2.2 mmol) with dichloromethane (2 ml) was added dropwise to the mixture. The reaction was stirred at 273 K for 2 h under an atmosphere of nitrogen and allowed to warm to room temperature over the course of 12 h, filtered, and the solvent removed by distillation under reduced pressure. The mixture was dissolved in EtOAc (60 ml), then was washed with 10% citric acid (40 ml), saturated $NaHCO_3$ (40 ml), and brine (40 ml), with backwashing. The combined organic extracts were dried ($NaSO_4$) and concentrated. The crude was purified by silica-gel chromatography with acetone-hexane (1:3) to give the title compound. Colorless crystals suitable for X-ray analysis (m.p.331 K) grew over a period of one week when the solution was exposed to air.

Refinement

Hydrogen atoms attached to C or N atoms were located at geometrically calculated positions [0.95 (CH), 0.99 (CH_2), 0.98 (CH_3), 0.88 (NH)] and refined with isotropic thermal parameters U_{iso}(H) equal to 1.2 for CH_2, CH, and NH, 1.5 for CH_3 U_{eq}(C atoms).

Figures

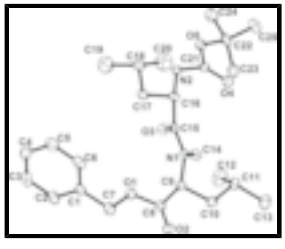


Fig. 1. The asymmetric unit of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Benzyl 2-{[2-(*tert*-butoxycarbonylamino)-4-methylpentanoyl]methylamino}- 4-methylpentanoate

Crystal data

$C_{25}H_{40}N_2O_5$	$D_x = 1.122$ Mg m^{-3}
$M_r = 448.59$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 13652 reflections
$a = 9.9400$ (12) Å	$\theta = 12$–18^o
$b = 14.9395$ (18) Å	$\mu = 0.08$ mm^{-1}
$c = 17.876$ (2) Å	$T = 173$ (2) K
$V = 2654.6$ (5) Å^3	Block, colourless
$Z = 4$	0.50 × 0.40 × 0.20 mm
$F_{000} = 976$	

Data collection

Bruker SMART 1000 CCD diffractometer	3277 independent reflections
Radiation source: fine-focus sealed tube	2732 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 173(2)$ K	$\theta_{max} = 27.1^o$
ω scans	$\theta_{min} = 2.3^o$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 12$
$T_{min} = 0.96$, $T_{max} = 0.99$	$k = -17 \rightarrow 19$
13652 measured reflections	$l = -22 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.6524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.099$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
3277 reflections	$\Delta\rho_{min} = -0.24$ e Å^{-3}
298 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983)
Secondary atom site location: difference Fourier map	Flack parameter: 0 (10)

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.12084 (16)	0.18042 (11)	0.90469 (9)	0.0411 (4)
O2	−0.03295 (18)	0.07107 (12)	0.90142 (9)	0.0455 (4)
O3	0.28053 (14)	0.19630 (10)	1.09159 (9)	0.0370 (4)
O4	0.13473 (17)	0.20856 (11)	1.26427 (9)	0.0442 (4)
O5	0.32332 (16)	0.28696 (10)	1.29608 (8)	0.0359 (3)
N1	0.06472 (18)	0.16720 (12)	1.05938 (9)	0.0294 (4)
N2	0.20996 (18)	0.32424 (11)	1.19348 (9)	0.0309 (4)
H2A	0.2604	0.3726	1.1918	0.037*
C1	0.1431 (2)	0.29670 (15)	0.81465 (11)	0.0356 (5)
C2	0.2561 (2)	0.29855 (17)	0.76974 (13)	0.0430 (6)
H2	0.2889	0.2446	0.7484	0.052*
C3	0.3219 (3)	0.37837 (19)	0.75561 (15)	0.0535 (7)
H3	0.4009	0.3789	0.7257	0.064*
C4	0.2730 (3)	0.45650 (18)	0.78484 (16)	0.0556 (7)
H4	0.3168	0.5115	0.7741	0.067*
C5	0.1610 (3)	0.45576 (18)	0.82960 (15)	0.0547 (7)
H5	0.1284	0.5102	0.8503	0.066*
C6	0.0957 (3)	0.37666 (18)	0.84466 (14)	0.0455 (6)
H6	0.0180	0.3766	0.8756	0.055*
C7	0.0715 (3)	0.21184 (19)	0.83221 (13)	0.0483 (6)
H7A	−0.0268	0.2224	0.8345	0.058*
H7B	0.0896	0.1666	0.7931	0.058*
C8	0.0554 (2)	0.11038 (15)	0.93323 (12)	0.0332 (5)
C9	0.1060 (2)	0.09157 (14)	1.01228 (12)	0.0312 (5)
H9	0.2066	0.0897	1.0110	0.037*
C10	0.0552 (3)	0.00139 (15)	1.04099 (13)	0.0386 (5)
H10A	−0.0443	0.0023	1.0407	0.046*
H10B	0.0846	−0.0458	1.0057	0.046*
C11	0.1025 (3)	−0.02395 (16)	1.11929 (14)	0.0421 (6)
H11	0.0708	0.0231	1.1550	0.051*
C12	0.2542 (3)	−0.0303 (2)	1.12513 (19)	0.0654 (9)
H12A	0.2794	−0.0458	1.1765	0.098*
H12B	0.2943	0.0275	1.1118	0.098*

H12C	0.2871	−0.0765	1.0909	0.098*
C13	0.0378 (3)	−0.11314 (18)	1.14157 (17)	0.0578 (7)
H13A	0.0685	−0.1603	1.1075	0.087*
H13B	−0.0603	−0.1079	1.1385	0.087*
H13C	0.0639	−0.1283	1.1929	0.087*
C14	−0.0782 (2)	0.19081 (16)	1.05734 (13)	0.0358 (5)
H14A	−0.0990	0.2310	1.0991	0.054*
H14B	−0.1326	0.1363	1.0616	0.054*
H14C	−0.0987	0.2209	1.0100	0.054*
C15	0.1613 (2)	0.21621 (14)	1.09387 (11)	0.0283 (4)
C16	0.1177 (2)	0.30299 (14)	1.13349 (11)	0.0305 (4)
H16	0.0252	0.2951	1.1544	0.037*
C17	0.1162 (2)	0.37809 (14)	1.07518 (12)	0.0350 (5)
H17A	0.2078	0.3836	1.0539	0.042*
H17B	0.0554	0.3601	1.0340	0.042*
C18	0.0725 (3)	0.46975 (15)	1.10310 (14)	0.0422 (6)
H18	0.1339	0.4868	1.1451	0.051*
C19	0.0895 (4)	0.53893 (19)	1.04158 (19)	0.0790 (11)
H19A	0.0306	0.5239	0.9995	0.118*
H19B	0.1833	0.5393	1.0247	0.118*
H19C	0.0657	0.5982	1.0609	0.118*
C20	−0.0700 (3)	0.4701 (2)	1.1334 (2)	0.0774 (10)
H20A	−0.0941	0.5309	1.1491	0.116*
H20B	−0.0759	0.4296	1.1764	0.116*
H20C	−0.1322	0.4501	1.0942	0.116*
C21	0.2165 (2)	0.26697 (14)	1.25290 (11)	0.0321 (5)
C22	0.3583 (3)	0.22819 (16)	1.36006 (12)	0.0393 (5)
C23	0.3851 (3)	0.13377 (16)	1.33291 (15)	0.0472 (6)
H23A	0.3015	0.1077	1.3136	0.071*
H23B	0.4184	0.0973	1.3746	0.071*
H23C	0.4526	0.1352	1.2930	0.071*
C24	0.4868 (3)	0.2711 (2)	1.38889 (14)	0.0510 (7)
H24A	0.5550	0.2707	1.3493	0.077*
H24B	0.5200	0.2374	1.4321	0.077*
H24C	0.4683	0.3330	1.4038	0.077*
C25	0.2492 (3)	0.2326 (2)	1.41909 (13)	0.0526 (7)
H25A	0.2336	0.2951	1.4332	0.079*
H25B	0.2775	0.1986	1.4632	0.079*
H25C	0.1659	0.2069	1.3991	0.079*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0439 (9)	0.0468 (9)	0.0326 (8)	−0.0112 (8)	−0.0077 (7)	0.0088 (7)
O2	0.0539 (10)	0.0452 (9)	0.0373 (9)	−0.0129 (8)	−0.0068 (8)	−0.0034 (8)
O3	0.0272 (7)	0.0380 (8)	0.0458 (9)	0.0041 (7)	−0.0032 (7)	−0.0059 (7)
O4	0.0431 (9)	0.0488 (9)	0.0407 (8)	−0.0132 (8)	−0.0019 (7)	0.0063 (8)
O5	0.0406 (8)	0.0360 (8)	0.0311 (7)	−0.0047 (7)	−0.0068 (7)	0.0043 (6)

N1	0.0287 (9)	0.0310 (9)	0.0284 (9)	0.0014 (7)	−0.0005 (7)	−0.0022 (7)
N2	0.0367 (10)	0.0289 (8)	0.0271 (8)	−0.0026 (8)	−0.0032 (8)	−0.0026 (7)
C1	0.0341 (11)	0.0461 (13)	0.0267 (10)	−0.0002 (10)	−0.0056 (9)	0.0064 (10)
C2	0.0451 (14)	0.0469 (13)	0.0369 (12)	0.0114 (12)	0.0053 (10)	0.0070 (11)
C3	0.0443 (14)	0.0694 (18)	0.0467 (14)	−0.0038 (14)	0.0087 (12)	0.0197 (14)
C4	0.0688 (18)	0.0471 (14)	0.0509 (15)	−0.0118 (14)	−0.0053 (15)	0.0139 (12)
C5	0.075 (2)	0.0459 (14)	0.0431 (14)	0.0111 (14)	−0.0044 (15)	0.0000 (12)
C6	0.0387 (13)	0.0632 (16)	0.0347 (12)	0.0113 (12)	0.0022 (10)	0.0015 (12)
C7	0.0532 (15)	0.0568 (15)	0.0347 (12)	−0.0120 (13)	−0.0110 (11)	0.0090 (12)
C8	0.0344 (11)	0.0342 (11)	0.0311 (11)	−0.0001 (10)	0.0021 (9)	−0.0032 (9)
C9	0.0326 (11)	0.0301 (10)	0.0308 (11)	0.0003 (9)	−0.0010 (9)	−0.0019 (9)
C10	0.0446 (13)	0.0311 (11)	0.0402 (12)	−0.0009 (10)	−0.0019 (11)	0.0005 (10)
C11	0.0517 (15)	0.0335 (11)	0.0410 (13)	0.0019 (11)	−0.0005 (11)	0.0062 (10)
C12	0.0542 (17)	0.0611 (18)	0.081 (2)	0.0023 (15)	−0.0153 (16)	0.0268 (17)
C13	0.0694 (18)	0.0442 (14)	0.0598 (17)	−0.0029 (14)	0.0034 (15)	0.0181 (13)
C14	0.0291 (11)	0.0427 (12)	0.0356 (11)	−0.0001 (10)	−0.0001 (9)	−0.0047 (10)
C15	0.0287 (10)	0.0298 (10)	0.0263 (9)	0.0005 (9)	−0.0009 (8)	0.0021 (8)
C16	0.0296 (10)	0.0344 (11)	0.0277 (10)	0.0023 (9)	−0.0031 (8)	−0.0029 (9)
C17	0.0430 (12)	0.0327 (11)	0.0291 (11)	0.0056 (10)	−0.0020 (9)	−0.0006 (9)
C18	0.0509 (14)	0.0367 (12)	0.0391 (12)	0.0109 (11)	−0.0098 (11)	−0.0039 (10)
C19	0.122 (3)	0.0391 (15)	0.076 (2)	0.0218 (18)	0.007 (2)	0.0129 (15)
C20	0.070 (2)	0.0630 (19)	0.099 (3)	0.0282 (18)	0.015 (2)	−0.0043 (19)
C21	0.0346 (11)	0.0328 (10)	0.0289 (10)	−0.0005 (10)	0.0000 (9)	−0.0040 (9)
C22	0.0455 (13)	0.0452 (13)	0.0273 (10)	0.0016 (11)	−0.0029 (10)	0.0074 (10)
C23	0.0542 (15)	0.0419 (13)	0.0455 (14)	0.0040 (12)	0.0051 (12)	0.0097 (11)
C24	0.0533 (15)	0.0618 (16)	0.0379 (12)	0.0003 (13)	−0.0126 (12)	0.0063 (12)
C25	0.0579 (16)	0.0675 (17)	0.0323 (12)	0.0099 (14)	0.0044 (11)	0.0084 (12)

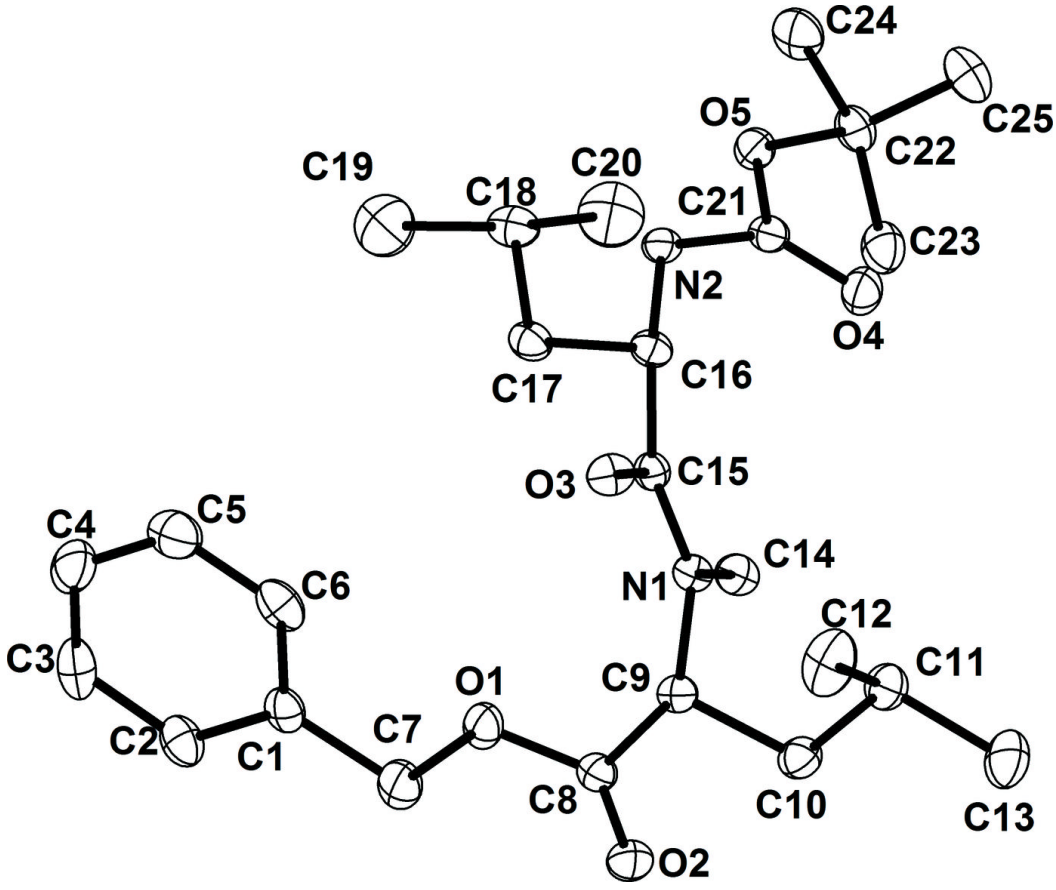
Geometric parameters (Å, °)

O1—C8	1.333 (3)	C12—H12A	0.9800
O1—C7	1.463 (3)	C12—H12B	0.9800
O2—C8	1.200 (3)	C12—H12C	0.9800
O3—C15	1.223 (2)	C13—H13A	0.9800
O4—C21	1.210 (3)	C13—H13B	0.9800
O5—C21	1.346 (3)	C13—H13C	0.9800
O5—C22	1.483 (3)	C14—H14A	0.9800
N1—C15	1.356 (3)	C14—H14B	0.9800
N1—C14	1.464 (3)	C14—H14C	0.9800
N1—C9	1.468 (3)	C15—C16	1.539 (3)
N2—C21	1.365 (3)	C16—C17	1.531 (3)
N2—C16	1.446 (3)	C16—H16	1.0000
N2—H2A	0.8800	C17—C18	1.521 (3)
C1—C2	1.381 (3)	C17—H17A	0.9900
C1—C6	1.392 (3)	C17—H17B	0.9900
C1—C7	1.488 (3)	C18—C20	1.517 (4)
C2—C3	1.383 (4)	C18—C19	1.519 (4)
C2—H2	0.9500	C18—H18	1.0000
C3—C4	1.368 (4)	C19—H19A	0.9800

C3—H3	0.9500	C19—H19B	0.9800
C4—C5	1.370 (4)	C19—H19C	0.9800
C4—H4	0.9500	C20—H20A	0.9800
C5—C6	1.375 (4)	C20—H20B	0.9800
C5—H5	0.9500	C20—H20C	0.9800
C6—H6	0.9500	C22—C25	1.514 (3)
C7—H7A	0.9900	C22—C23	1.515 (3)
C7—H7B	0.9900	C22—C24	1.519 (4)
C8—C9	1.526 (3)	C23—H23A	0.9800
C9—C10	1.528 (3)	C23—H23B	0.9800
C9—H9	1.0000	C23—H23C	0.9800
C10—C11	1.524 (3)	C24—H24A	0.9800
C10—H10A	0.9900	C24—H24B	0.9800
C10—H10B	0.9900	C24—H24C	0.9800
C11—C12	1.515 (4)	C25—H25A	0.9800
C11—C13	1.532 (3)	C25—H25B	0.9800
C11—H11	1.0000	C25—H25C	0.9800
C8—O1—C7	115.28 (18)	N1—C14—H14B	109.5
C21—O5—C22	119.72 (17)	H14A—C14—H14B	109.5
C15—N1—C14	124.62 (18)	N1—C14—H14C	109.5
C15—N1—C9	118.60 (18)	H14A—C14—H14C	109.5
C14—N1—C9	116.28 (18)	H14B—C14—H14C	109.5
C21—N2—C16	118.01 (17)	O3—C15—N1	122.7 (2)
C21—N2—H2A	121.0	O3—C15—C16	119.51 (18)
C16—N2—H2A	121.0	N1—C15—C16	117.73 (18)
C2—C1—C6	118.8 (2)	N2—C16—C17	110.50 (17)
C2—C1—C7	121.9 (2)	N2—C16—C15	110.36 (16)
C6—C1—C7	119.2 (2)	C17—C16—C15	107.86 (16)
C1—C2—C3	120.5 (2)	N2—C16—H16	109.4
C1—C2—H2	119.7	C17—C16—H16	109.4
C3—C2—H2	119.7	C15—C16—H16	109.4
C4—C3—C2	119.8 (2)	C18—C17—C16	116.04 (18)
C4—C3—H3	120.1	C18—C17—H17A	108.3
C2—C3—H3	120.1	C16—C17—H17A	108.3
C3—C4—C5	120.3 (3)	C18—C17—H17B	108.3
C3—C4—H4	119.8	C16—C17—H17B	108.3
C5—C4—H4	119.8	H17A—C17—H17B	107.4
C4—C5—C6	120.3 (3)	C20—C18—C19	111.1 (3)
C4—C5—H5	119.8	C20—C18—C17	112.8 (2)
C6—C5—H5	119.8	C19—C18—C17	110.1 (2)
C5—C6—C1	120.1 (2)	C20—C18—H18	107.5
C5—C6—H6	119.9	C19—C18—H18	107.5
C1—C6—H6	119.9	C17—C18—H18	107.5
O1—C7—C1	107.45 (19)	C18—C19—H19A	109.5
O1—C7—H7A	110.2	C18—C19—H19B	109.5
C1—C7—H7A	110.2	H19A—C19—H19B	109.5
O1—C7—H7B	110.2	C18—C19—H19C	109.5
C1—C7—H7B	110.2	H19A—C19—H19C	109.5
H7A—C7—H7B	108.5	H19B—C19—H19C	109.5

O2—C8—O1	124.0 (2)	C18—C20—H20A	109.5
O2—C8—C9	126.2 (2)	C18—C20—H20B	109.5
O1—C8—C9	109.76 (18)	H20A—C20—H20B	109.5
N1—C9—C8	107.28 (17)	C18—C20—H20C	109.5
N1—C9—C10	113.18 (18)	H20A—C20—H20C	109.5
C8—C9—C10	111.39 (18)	H20B—C20—H20C	109.5
N1—C9—H9	108.3	O4—C21—O5	126.4 (2)
C8—C9—H9	108.3	O4—C21—N2	123.4 (2)
C10—C9—H9	108.3	O5—C21—N2	110.16 (18)
C11—C10—C9	115.2 (2)	O5—C22—C25	110.11 (19)
C11—C10—H10A	108.5	O5—C22—C23	110.19 (18)
C9—C10—H10A	108.5	C25—C22—C23	112.9 (2)
C11—C10—H10B	108.5	O5—C22—C24	102.04 (19)
C9—C10—H10B	108.5	C25—C22—C24	110.3 (2)
H10A—C10—H10B	107.5	C23—C22—C24	110.7 (2)
C12—C11—C10	112.7 (2)	C22—C23—H23A	109.5
C12—C11—C13	110.2 (2)	C22—C23—H23B	109.5
C10—C11—C13	109.0 (2)	H23A—C23—H23B	109.5
C12—C11—H11	108.3	C22—C23—H23C	109.5
C10—C11—H11	108.3	H23A—C23—H23C	109.5
C13—C11—H11	108.3	H23B—C23—H23C	109.5
C11—C12—H12A	109.5	C22—C24—H24A	109.5
C11—C12—H12B	109.5	C22—C24—H24B	109.5
H12A—C12—H12B	109.5	H24A—C24—H24B	109.5
C11—C12—H12C	109.5	C22—C24—H24C	109.5
H12A—C12—H12C	109.5	H24A—C24—H24C	109.5
H12B—C12—H12C	109.5	H24B—C24—H24C	109.5
C11—C13—H13A	109.5	C22—C25—H25A	109.5
C11—C13—H13B	109.5	C22—C25—H25B	109.5
H13A—C13—H13B	109.5	H25A—C25—H25B	109.5
C11—C13—H13C	109.5	C22—C25—H25C	109.5
H13A—C13—H13C	109.5	H25A—C25—H25C	109.5
H13B—C13—H13C	109.5	H25B—C25—H25C	109.5
N1—C14—H14A	109.5		

Fig. 1


C24
C25
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C14
C6
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C12
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C9
C11
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C7
C8
C10
C13
O2