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1-(*tert*-Butoxycarbonyl)piperidine-4-carboxylic acidHoong-Kun Fun,^{a,*} Suhana Arshad,^a Dinesh,^b S. Vivek^b and G. K. Nagaraja^b^aX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and ^bDepartment of Chemistry, Mangalore University, Karnataka, India

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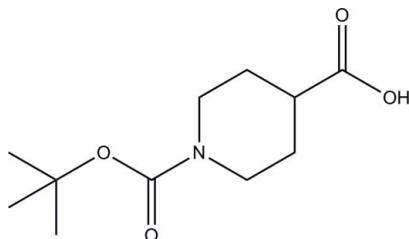
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.039; wR factor = 0.092; data-to-parameter ratio = 13.9.

In the title compound, $\text{C}_{11}\text{H}_{19}\text{NO}_4$, the piperidine ring adopts a chair conformation. In the crystal, molecules are linked by intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a layer parallel to the bc plane.

Related literature

For general background and application of helical peptides, see: Albrecht & Stortz (2005); Garner & Harding (2007); Wang *et al.* (2008); Walensky *et al.* (2004); Boal *et al.* (2007). For bond-length data, see: Allen *et al.* (1987). For ring conformations, see: Cremer & Pople (1975). For stability of the temperature controller used for data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$\text{C}_{11}\text{H}_{19}\text{NO}_4$
 $M_r = 229.27$
 Monoclinic, $P2_1/c$
 $a = 10.7006$ (3) Å

$b = 6.5567$ (2) Å
 $c = 17.9297$ (6) Å
 $\beta = 104.564$ (2)°
 $V = 1217.54$ (6) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹

$T = 100$ K
 $0.57 \times 0.21 \times 0.08$ mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.948$, $T_{\max} = 0.993$

5360 measured reflections
 2116 independent reflections
 1762 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.092$
 $S = 1.07$
 2116 reflections
 152 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|----------|-------------|-------------|---------------|
| $\text{O4}-\text{H1O4}\cdots\text{O1}^i$ | 0.86 (2) | 1.82 (2) | 2.6562 (16) | 164 (2) |
| $\text{C5}-\text{H5B}\cdots\text{O4}^{ii}$ | 0.99 | 2.56 | 3.476 (2) | 154 |

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2754).

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supplementary materials

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1-(*tert*-Butoxycarbonyl)piperidine-4-carboxylic acid

H.-K. Fun, S. Arshad, Dinesh, S. Vivek and G. K. Nagaraja

Comment

An intramolecular side-chain metal ligation is a useful method for stabilizing β -sheet, turn and helical structures in short peptides (Albrecht & Stortz, 2005; Garner & Harding, 2007). The stabilization of helical structure may enhance biological activities and protease resistance *in vitro* or *in vivo* (Wang *et al.*, 2008; Walensky *et al.*, 2004). The present compound, 1-(*tert*-butoxycarbonyl)piperidine-4-carboxylic acid, may be used as a rigid backbone to design the metal-ligating 3_{10} -helical peptide. In this way we may be able to design, synthesize and characterize a dynamically optically inactive 3_{10} -helical peptide which possess a metal-chelating ability (Boal *et al.*, 2007).

In the molecular structure (Fig. 1), the piperidine ring (N1/C1–C5) adopts a chair conformation with puckering amplitude $Q = 0.5505$ (16) Å, $\Theta = 179.17$ (18) $^\circ$ and $\varphi = 90$ (11) $^\circ$ (Cremer & Pople, 1975). The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges.

The crystal packing is shown in Fig. 2. The molecules are linked by intermolecular O4—H1O4 \cdots O1 and C5—H5B \cdots O4 (Table 1) hydrogen bonds, forming two-molecular sheets parallel to the *bc* plane.

Experimental

To isopicotinic acid (1 eq) dissolved in a dichloromethane (10 ml), triethylamine (3 eq) was added. The reaction mixture was stirred at room temperature for half an hour. BOC-anhydride (2 eq) was then added and the reaction mixture heated at 40 $^\circ$ C for 12 h. Completion of the reaction was confirmed by TLC and the solvent content was evaporated away under reduced pressure. The reaction mixture was acidified with diluted. HCl and the solid obtained was filtered off. *M. p.*: 135–137 $^\circ$ C.

Refinement

H1O4 atom attached to the O atom was located in a difference map and refined freely [O—H = 0.86 (2) Å]. The remaining H atoms were positioned geometrically (C—H = 0.98–1.00 Å) and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$. A rotating group model was applied to the methyl groups.

Figures

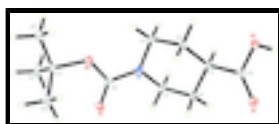


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.



Fig. 2. The crystal packing of the title compound showing a two-molecular thick sheet. Dashed lines represent the intermolecular hydrogen bonds.

1-(*tert*-Butoxycarbonyl)piperidine-4-carboxylic acid

Crystal data

| | |
|---------------------------------|---|
| $C_{11}H_{19}NO_4$ | $F(000) = 496$ |
| $M_r = 229.27$ | $D_x = 1.251 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: -P 2ybc | Cell parameters from 1750 reflections |
| $a = 10.7006 (3) \text{ \AA}$ | $\theta = 2.4\text{--}28.5^\circ$ |
| $b = 6.5567 (2) \text{ \AA}$ | $\mu = 0.10 \text{ mm}^{-1}$ |
| $c = 17.9297 (6) \text{ \AA}$ | $T = 100 \text{ K}$ |
| $\beta = 104.564 (2)^\circ$ | Plate, colourless |
| $V = 1217.54 (6) \text{ \AA}^3$ | $0.57 \times 0.21 \times 0.08 \text{ mm}$ |
| $Z = 4$ | |

Data collection

| | |
|---|--|
| Bruker SMART APEXII CCD area-detector diffractometer | 2116 independent reflections |
| Radiation source: fine-focus sealed tube graphite | 1762 reflections with $I > 2\sigma(I)$ |
| φ and ω scans | $R_{\text{int}} = 0.027$ |
| Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2009) | $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.0^\circ$ |
| $T_{\text{min}} = 0.948$, $T_{\text{max}} = 0.993$ | $h = -12 \rightarrow 11$ |
| 5360 measured reflections | $k = -7 \rightarrow 7$ |
| | $l = -16 \rightarrow 21$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.092$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.07$ | $w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 0.3737P]$ |
| 2116 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 152 parameters | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 0 restraints | $\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$ |

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|---------------|--------------|----------------------------------|
| O1 | 0.26358 (11) | -0.05214 (18) | 0.13924 (6) | 0.0249 (3) |
| O2 | 0.20095 (11) | 0.21800 (16) | 0.20083 (6) | 0.0229 (3) |
| O3 | 0.34156 (12) | -0.53547 (17) | 0.46087 (7) | 0.0265 (3) |
| O4 | 0.35972 (11) | -0.25776 (18) | 0.53522 (6) | 0.0244 (3) |
| N1 | 0.34480 (13) | -0.0015 (2) | 0.26790 (7) | 0.0188 (3) |
| C1 | 0.42896 (16) | -0.1805 (2) | 0.27802 (9) | 0.0213 (4) |
| H1A | 0.5202 | -0.1364 | 0.2948 | 0.026* |
| H1B | 0.4167 | -0.2525 | 0.2282 | 0.026* |
| C2 | 0.39922 (16) | -0.3257 (2) | 0.33783 (9) | 0.0195 (4) |
| H2A | 0.4628 | -0.4385 | 0.3473 | 0.023* |
| H2B | 0.3123 | -0.3855 | 0.3176 | 0.023* |
| C3 | 0.40397 (15) | -0.2158 (2) | 0.41359 (9) | 0.0178 (4) |
| H3A | 0.4949 | -0.1705 | 0.4361 | 0.021* |
| C4 | 0.31744 (15) | -0.0254 (2) | 0.39936 (9) | 0.0186 (4) |
| H4A | 0.2259 | -0.0677 | 0.3819 | 0.022* |
| H4B | 0.3284 | 0.0509 | 0.4482 | 0.022* |
| C5 | 0.35063 (16) | 0.1126 (2) | 0.33908 (9) | 0.0202 (4) |
| H5A | 0.2891 | 0.2280 | 0.3280 | 0.024* |
| H5B | 0.4385 | 0.1690 | 0.3591 | 0.024* |
| C6 | 0.26959 (15) | 0.0473 (2) | 0.19822 (9) | 0.0190 (4) |
| C7 | 0.10863 (15) | 0.2991 (3) | 0.13127 (9) | 0.0221 (4) |
| C8 | 0.06014 (17) | 0.4903 (3) | 0.16286 (10) | 0.0288 (4) |
| H8A | 0.0189 | 0.4528 | 0.2039 | 0.043* |
| H8B | -0.0027 | 0.5596 | 0.1214 | 0.043* |
| H8C | 0.1330 | 0.5818 | 0.1837 | 0.043* |
| C9 | 0.17864 (18) | 0.3540 (3) | 0.07020 (10) | 0.0330 (5) |
| H9A | 0.2538 | 0.4391 | 0.0932 | 0.049* |
| H9B | 0.1201 | 0.4294 | 0.0285 | 0.049* |
| H9C | 0.2073 | 0.2291 | 0.0495 | 0.049* |
| C10 | 0.00063 (17) | 0.1463 (3) | 0.10281 (10) | 0.0303 (4) |
| H10A | -0.0400 | 0.1137 | 0.1446 | 0.046* |
| H10B | 0.0361 | 0.0215 | 0.0861 | 0.046* |
| H10C | -0.0639 | 0.2048 | 0.0594 | 0.046* |
| C11 | 0.36557 (14) | -0.3565 (2) | 0.47085 (9) | 0.0183 (4) |
| H104 | 0.333 (2) | -0.340 (4) | 0.5652 (13) | 0.058 (7)* |

supplementary materials

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|------------|-------------|
| O1 | 0.0329 (7) | 0.0282 (7) | 0.0148 (6) | 0.0004 (5) | 0.0084 (5) | -0.0034 (5) |
| O2 | 0.0274 (6) | 0.0221 (6) | 0.0170 (6) | 0.0056 (5) | 0.0018 (5) | 0.0005 (5) |
| O3 | 0.0390 (7) | 0.0190 (7) | 0.0240 (7) | -0.0008 (5) | 0.0125 (6) | 0.0008 (5) |
| O4 | 0.0353 (7) | 0.0226 (7) | 0.0175 (6) | -0.0008 (5) | 0.0109 (6) | 0.0003 (5) |
| N1 | 0.0264 (8) | 0.0164 (7) | 0.0138 (7) | 0.0028 (6) | 0.0056 (6) | 0.0008 (6) |
| C1 | 0.0253 (9) | 0.0206 (9) | 0.0201 (9) | 0.0064 (7) | 0.0099 (7) | -0.0003 (7) |
| C2 | 0.0234 (9) | 0.0174 (8) | 0.0191 (9) | 0.0044 (7) | 0.0082 (7) | 0.0014 (7) |
| C3 | 0.0181 (8) | 0.0183 (9) | 0.0168 (8) | -0.0005 (7) | 0.0043 (7) | 0.0012 (7) |
| C4 | 0.0218 (9) | 0.0189 (9) | 0.0153 (8) | 0.0010 (7) | 0.0051 (7) | -0.0019 (7) |
| C5 | 0.0271 (9) | 0.0166 (8) | 0.0164 (8) | 0.0002 (7) | 0.0048 (7) | -0.0011 (7) |
| C6 | 0.0215 (9) | 0.0184 (9) | 0.0190 (9) | -0.0017 (7) | 0.0086 (7) | 0.0033 (7) |
| C7 | 0.0205 (9) | 0.0276 (9) | 0.0159 (8) | 0.0012 (7) | 0.0006 (7) | 0.0046 (7) |
| C8 | 0.0264 (10) | 0.0274 (10) | 0.0296 (10) | 0.0053 (8) | 0.0017 (8) | 0.0026 (8) |
| C9 | 0.0311 (10) | 0.0395 (11) | 0.0297 (10) | 0.0074 (9) | 0.0101 (8) | 0.0152 (9) |
| C10 | 0.0257 (10) | 0.0341 (11) | 0.0295 (10) | -0.0009 (8) | 0.0039 (8) | -0.0021 (8) |
| C11 | 0.0167 (8) | 0.0204 (9) | 0.0170 (8) | 0.0034 (7) | 0.0025 (7) | -0.0003 (7) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------------|-------------|------------|-------------|
| O1—C6 | 1.2303 (18) | C4—C5 | 1.519 (2) |
| O2—C6 | 1.3457 (19) | C4—H4A | 0.9900 |
| O2—C7 | 1.4815 (18) | C4—H4B | 0.9900 |
| O3—C11 | 1.2050 (19) | C5—H5A | 0.9900 |
| O4—C11 | 1.3384 (18) | C5—H5B | 0.9900 |
| O4—H104 | 0.86 (2) | C7—C9 | 1.517 (2) |
| N1—C6 | 1.344 (2) | C7—C10 | 1.518 (2) |
| N1—C1 | 1.463 (2) | C7—C8 | 1.519 (2) |
| N1—C5 | 1.4669 (19) | C8—H8A | 0.9800 |
| C1—C2 | 1.526 (2) | C8—H8B | 0.9800 |
| C1—H1A | 0.9900 | C8—H8C | 0.9800 |
| C1—H1B | 0.9900 | C9—H9A | 0.9800 |
| C2—C3 | 1.527 (2) | C9—H9B | 0.9800 |
| C2—H2A | 0.9900 | C9—H9C | 0.9800 |
| C2—H2B | 0.9900 | C10—H10A | 0.9800 |
| C3—C11 | 1.512 (2) | C10—H10B | 0.9800 |
| C3—C4 | 1.537 (2) | C10—H10C | 0.9800 |
| C3—H3A | 1.0000 | | |
| C6—O2—C7 | 121.57 (12) | C4—C5—H5B | 109.6 |
| C11—O4—H104 | 109.2 (15) | H5A—C5—H5B | 108.1 |
| C6—N1—C1 | 120.84 (13) | O1—C6—N1 | 124.22 (15) |
| C6—N1—C5 | 124.88 (13) | O1—C6—O2 | 124.04 (15) |
| C1—N1—C5 | 114.27 (12) | N1—C6—O2 | 111.74 (13) |
| N1—C1—C2 | 110.93 (12) | O2—C7—C9 | 110.31 (13) |
| N1—C1—H1A | 109.5 | O2—C7—C10 | 109.63 (13) |

| | | | |
|--------------|--------------|---------------|--------------|
| C2—C1—H1A | 109.5 | C9—C7—C10 | 112.73 (15) |
| N1—C1—H1B | 109.5 | O2—C7—C8 | 101.56 (12) |
| C2—C1—H1B | 109.5 | C9—C7—C8 | 110.50 (14) |
| H1A—C1—H1B | 108.0 | C10—C7—C8 | 111.56 (14) |
| C1—C2—C3 | 111.36 (13) | C7—C8—H8A | 109.5 |
| C1—C2—H2A | 109.4 | C7—C8—H8B | 109.5 |
| C3—C2—H2A | 109.4 | H8A—C8—H8B | 109.5 |
| C1—C2—H2B | 109.4 | C7—C8—H8C | 109.5 |
| C3—C2—H2B | 109.4 | H8A—C8—H8C | 109.5 |
| H2A—C2—H2B | 108.0 | H8B—C8—H8C | 109.5 |
| C11—C3—C2 | 111.22 (13) | C7—C9—H9A | 109.5 |
| C11—C3—C4 | 110.67 (12) | C7—C9—H9B | 109.5 |
| C2—C3—C4 | 110.60 (13) | H9A—C9—H9B | 109.5 |
| C11—C3—H3A | 108.1 | C7—C9—H9C | 109.5 |
| C2—C3—H3A | 108.1 | H9A—C9—H9C | 109.5 |
| C4—C3—H3A | 108.1 | H9B—C9—H9C | 109.5 |
| C5—C4—C3 | 111.29 (12) | C7—C10—H10A | 109.5 |
| C5—C4—H4A | 109.4 | C7—C10—H10B | 109.5 |
| C3—C4—H4A | 109.4 | H10A—C10—H10B | 109.5 |
| C5—C4—H4B | 109.4 | C7—C10—H10C | 109.5 |
| C3—C4—H4B | 109.4 | H10A—C10—H10C | 109.5 |
| H4A—C4—H4B | 108.0 | H10B—C10—H10C | 109.5 |
| N1—C5—C4 | 110.43 (12) | O3—C11—O4 | 122.99 (15) |
| N1—C5—H5A | 109.6 | O3—C11—C3 | 125.29 (14) |
| C4—C5—H5A | 109.6 | O4—C11—C3 | 111.72 (13) |
| N1—C5—H5B | 109.6 | | |
| C6—N1—C1—C2 | -123.01 (15) | C1—N1—C6—O2 | -179.20 (13) |
| C5—N1—C1—C2 | 56.56 (17) | C5—N1—C6—O2 | 1.3 (2) |
| N1—C1—C2—C3 | -53.55 (17) | C7—O2—C6—O1 | 1.2 (2) |
| C1—C2—C3—C11 | 176.11 (13) | C7—O2—C6—N1 | -178.49 (13) |
| C1—C2—C3—C4 | 52.71 (17) | C6—O2—C7—C9 | -61.40 (18) |
| C11—C3—C4—C5 | -177.27 (13) | C6—O2—C7—C10 | 63.30 (17) |
| C2—C3—C4—C5 | -53.56 (17) | C6—O2—C7—C8 | -178.59 (13) |
| C6—N1—C5—C4 | 122.38 (16) | C2—C3—C11—O3 | 4.2 (2) |
| C1—N1—C5—C4 | -57.18 (17) | C4—C3—C11—O3 | 127.55 (17) |
| C3—C4—C5—N1 | 54.71 (17) | C2—C3—C11—O4 | -175.19 (13) |
| C1—N1—C6—O1 | 1.1 (2) | C4—C3—C11—O4 | -51.83 (17) |
| C5—N1—C6—O1 | -178.39 (14) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|----------|-------------|-------------|---------------|
| O4—H10A \cdots O1 ⁱ | 0.86 (2) | 1.82 (2) | 2.6562 (16) | 164 (2) |
| C5—H5B \cdots O4 ⁱⁱ | 0.99 | 2.56 | 3.476 (2) | 154. |

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

Fig. 1

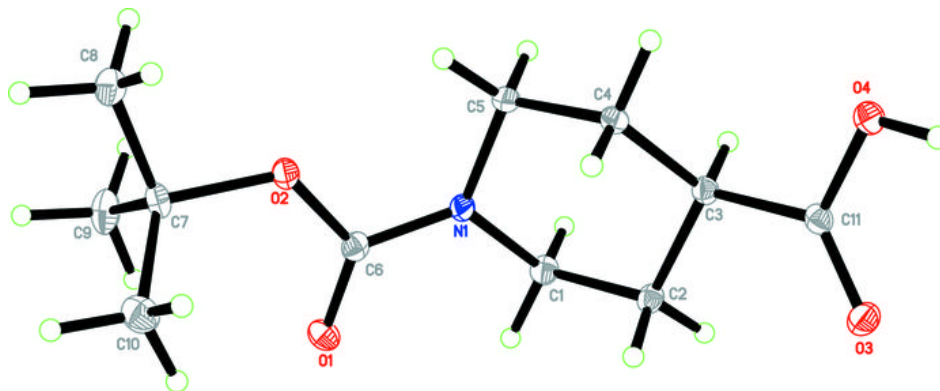


Fig. 2

