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Cyclo(alanine-4-hydroxyproline)

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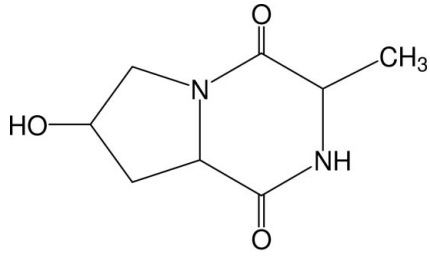
The title compound, 2-hydroxy-6-methyl-1,2,3,5,6,7,8,8a-octahydro-7-azaindolizine-5,8-dione, $C_8H_{12}N_2O_2$, is bicyclic. The six-membered ring has a boat configuration. The five-membered ring shares one of the prow points and is hinged towards the open part of the boat. Together the rings appear to adopt a slight dish shape. The methyl group is on the open-dish side and the hydroxyl group is *trans* to it. Hydrogen bonds in the crystal knit molecules into corrugated layers.

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.096
Data-to-parameter ratio = 9.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



(I)

Experimental

The title compound was prepared and recrystallized by Zeng (2000) according to the following procedure: L-*trans* 4-hydroxyproline (with nitrogen protected) and L-alanine methyl ester hydrochloride were reacted in 1:1 chloroform/acetronitrile following the method of Carpino *et al.* (1986). The reaction was quenched with water and normal work-up of the organic layer afforded the title compound. Crystals were obtained from chloroform solution.

Crystal data

$C_8H_{12}N_2O_3$
M_r = 184.20
Monoclinic, $P2_1$
a = 8.626 (2) Å
b = 9.924 (3) Å
c = 5.179 (1) Å
β = 103.719 (9)°
V = 430.70 (18) Å^3
Z = 2
D_x = 1.420 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 16 reflections
θ = 11–13°
μ = 0.11 mm^{-1}
T = 293 (2) K
Prism, colorless
0.45 × 0.30 × 0.20 mm

Data collection

Picker four-circle diffractometer
$\theta/2\theta$ scans
2100 measured reflections
1099 independent reflections
835 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.0°
$h = -9 \rightarrow 11$
$k = -10 \rightarrow 13$
$l = -6 \rightarrow 4$
3 standard reflections every 150 reflections
intensity decay: <1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0264P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.096$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$S = 0.99$	$\Delta\rho_{min} = -0.18$ e Å^{-3}
1099 reflections	Extinction correction: *SHELXL*97
120 parameters	Extinction coefficient: 0.074 (13)
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.10	2.945 (3)	165
O3—H3···O1^{ii}	0.82	1.97	2.761 (3)	163

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

Friedel-pair reflections were merged before final refinement because molybdenum radiation was employed and no atoms heavier than silicon are present in this structure. The absolute structure parameter (Flack parameter and its associated error) was −1.0 with an s.u. of 18.

Data collection: *XSTAL* (Brown, 1985), a modification of Picker FACS-I software (Picker, 1967); cell refinement: *CELL* (Brown, 1985); data reduction: *MINCON* (Brown, 1985); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997).

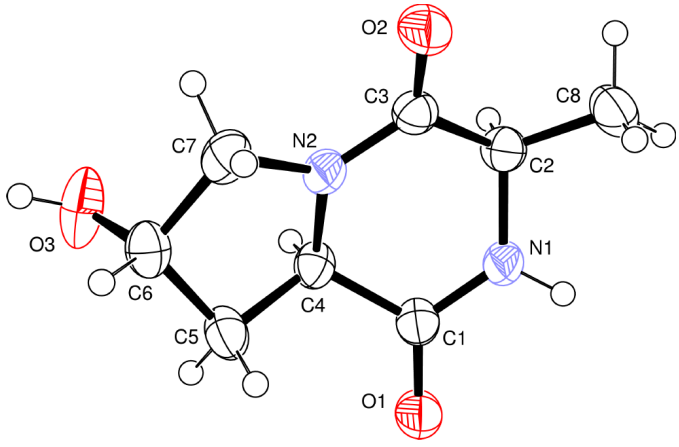


Figure 1
The structure of (I) showing 50% displacement ellipsoids.

References

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