# Crystal structure of (*S*)-2-(2-oxopyrrolidin-1-yl)butanoic acid, $C_8H_{13}NO_3$

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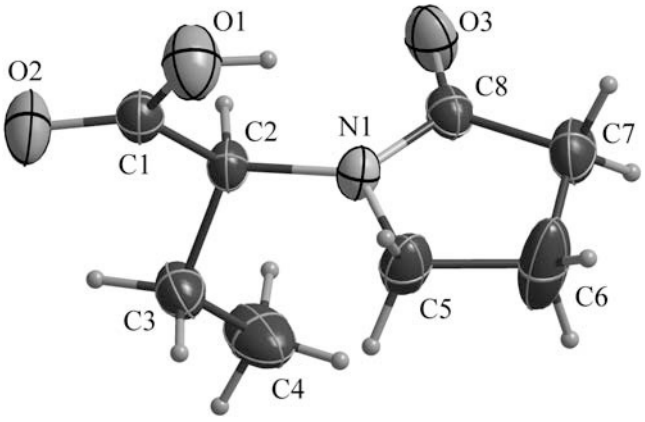


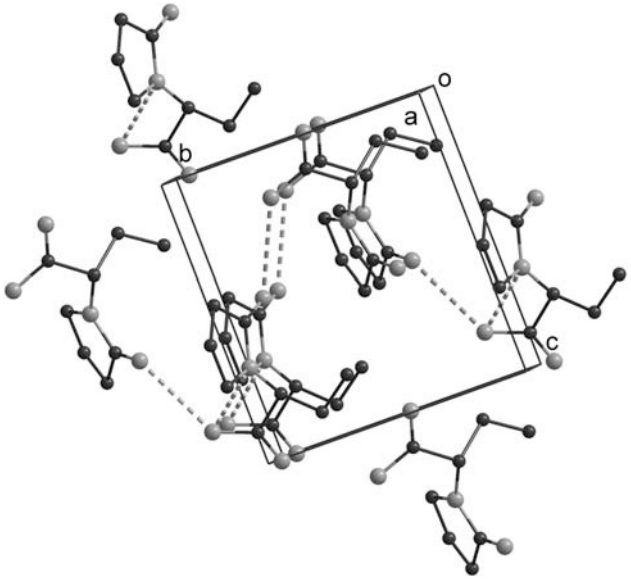


**Abstract**

$C_8H_{13}NO_3$, monoclinic, $P2_1$ (no. 4), $a$ = 6.285(3) Å, $b$ = 8.010(4) Å, $c$ = 9.190(5) Å, $\beta$ = 108.411(7)°, $V$ = 439.0 Å$^3$, $Z$ = 2, $R_{gf}(F)$ = 0.046, $wR_{ref}(F^2)$ = 0.132, $T$ = 293 K.

**Source of material**

(*S*)- 2-(2-oxopyrrolidin-1-yl)butanoic acid of analytical purity grade was obtained commercially. Crystals of the title compound were acquired after 0.171 g (0.001 mol) (*S*)-2-(2-oxopyrrolidin-1-yl)butanoic acid recrystallized from 25 ml ethanol by slow of solvent evaporation in air.

**Experimental details**

All H atoms were located at calculated positions and refined as riding on their parent atoms with the bond length fixed to 0.97 Å (methylene), 0.96 Å (methyl) and 0.82 Å (hydroxyl) and with $U_{iso}$(H) being 1.2 $U_{eq}$(C) with the exception of $U_{iso}$(H) being 1.5 $U_{eq}$(O and C for methyl group). The Flack parameter value is $x$ = 0.9(17).

**Discussion**

The molecule $C_8H_{13}NO_3$ was determined to be in *S* absolute configuration (figure, top). In the molecule there is a five-member lactam ring C5, C6, C7, C8 and N1, of which all five members in addtion to atoms O3 and C2 are approximately coplanar, the mean and maximum deviation from the least-squares plane through all relevant atoms being 0.078 Å and 0.153 Å for atom C6, respectively. All geometric parameters in the structure are in normal range. In addition to intra-molecular hydrogen bond of O1–H···N1, which consolidating the molecules' space configuration, the intermolecular hydrogen bond of O1–H···O3 (symmetry code: $-x$+2,$y$+1/2,$-z$+1) connects adjacent discrete molecules to zigzag chains along [010], which are further stack together to be a 3D framework (figure, bottom).

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | colorless block, size 0.320 × 0.350 × 0.420 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 0.99 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART CCD, $\varphi/\omega$ |
| $2\theta_{max}$: | 52° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 2807, 1620 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 1548 |
| $N(param)_{refined}$: | 111 |
| Programs: | SHELXS-97 [1], SHELXL-97 [2], SHELXTL [3], DIAMOND [4] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1) | 2*a* | 0.9233 | 0.6491 | 0.2474 | 0.079 |
| H(2) | 2*a* | 0.9839 | 0.2934 | 0.2622 | 0.034 |
| H(5A) | 2*a* | 0.4336 | 0.4561 | 0.2146 | 0.052 |
| H(5B) | 2*a* | 0.5644 | 0.6266 | 0.2594 | 0.052 |
| H(3A) | 2*a* | 0.5482 | 0.2883 | 0.0465 | 0.047 |
| H(3B) | 2*a* | 0.7507 | 0.1820 | 0.0336 | 0.047 |
| H(7A) | 2*a* | 0.6859 | 0.3804 | 0.6333 | 0.050 |
| H(7B) | 2*a* | 0.7909 | 0.5571 | 0.6223 | 0.050 |
| H(4A) | 2*a* | 0.7555 | 0.0436 | 0.2639 | 0.088 |

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**Table 2.** Continued.

| Atom | Site | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|
| H(4B) | 2*a* | 0.5374 | 0.0085 | 0.1267 | 0.088 |
| H(4C) | 2*a* | 0.5324 | 0.1369 | 0.2541 | 0.088 |
| H(6A) | 2*a* | 0.4587 | 0.6227 | 0.4653 | 0.086 |
| H(6B) | 2*a* | 0.3846 | 0.4342 | 0.4397 | 0.086 |

**Table 3.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| O(1) | 2*a* | 0.9458(4) | 0.6459(3) | 0.1643(2) | 0.072(1) | 0.043(1) | 0.050(1) | –0.005(1) | 0.029(1) | –0.0033(9) |
| O(2) | 2*a* | 0.9549(4) | 0.4482(2) | –0.0061(2) | 0.071(1) | 0.041(1) | 0.0428(9) | –0.0080(9) | 0.0368(9) | –0.0052(8) |
| O(3) | 2*a* | 1.0293(3) | 0.3021(3) | 0.5288(2) | 0.050(1) | 0.048(1) | 0.0287(8) | 0.0103(9) | 0.0097(7) | 0.0048(7) |
| N(1) | 2*a* | 0.7649(3) | 0.4243(2) | 0.3264(2) | 0.032(1) | 0.0315(9) | 0.0255(9) | 0.0021(7) | 0.0135(7) | 0.0020(7) |
| C(8) | 2*a* | 0.8585(4) | 0.3852(3) | 0.4766(2) | 0.040(1) | 0.029(1) | 0.027(1) | –0.005(1) | 0.0128(9) | –0.0013(9) |
| C(2) | 2*a* | 0.8482(4) | 0.3564(3) | 0.2085(2) | 0.033(1) | 0.029(1) | 0.025(1) | 0.0001(9) | 0.0135(8) | –0.0021(8) |
| C(1) | 2*a* | 0.9203(4) | 0.4902(3) | 0.1118(3) | 0.035(1) | 0.034(1) | 0.029(1) | –0.0007(9) | 0.0132(9) | –0.0019(9) |
| C(5) | 2*a* | 0.5513(5) | 0.5133(4) | 0.2932(3) | 0.037(1) | 0.056(2) | 0.040(1) | 0.013(1) | 0.017(1) | 0.003(1) |
| C(3) | 2*a* | 0.6833(5) | 0.2301(3) | 0.1054(3) | 0.049(1) | 0.040(1) | 0.032(1) | –0.009(1) | 0.015(1) | –0.006(1) |
| C(7) | 2*a* | 0.7164(5) | 0.4612(3) | 0.5637(3) | 0.054(2) | 0.041(1) | 0.036(1) | –0.005(1) | 0.025(1) | –0.007(1) |
| C(4) | 2*a* | 0.6216(6) | 0.0924(4) | 0.1957(4) | 0.072(2) | 0.050(2) | 0.049(2) | –0.027(2) | 0.014(2) | –0.003(1) |
| C(6) | 2*a* | 0.5041(7) | 0.5124(6) | 0.4432(4) | 0.068(2) | 0.107(3) | 0.054(2) | 0.047(2) | 0.039(2) | 0.023(2) |

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## References

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