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S-Benzyl-L-cysteine

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S-Benzyl-L-cysteine, $C_{10}H_{13}NO_2S$, contains two molecules in the asymmetric unit, both of which are zwitterions. They differ principally in terms of molecular conformation about their $C\alpha-C\beta$ bonds; one is approximately *anti*, the other *gauche* for the N—C—C—S grouping. The N—H···O hydrogen-bonding scheme has been elucidated.

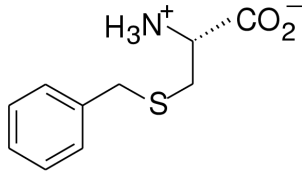
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.062
wR factor = 0.160
Data-to-parameter ratio = 18.4

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

Comment

S-Benzyl-L-cysteine, (I), was prepared as part of our studies into synthetic routes to derivatives of the potent cytotoxic agent thiocoraline (Boger *et al.*, 2001).



(I)

The geometrical parameters of the two distinct molecules are normal [d_{av}(S—C) = 1.819 (4) Å]. Their conformations differ principally in terms of the torsion angles about their $C\alpha-C\beta$ bonds (Fig. 1 and Table 1). The first (S1) molecule

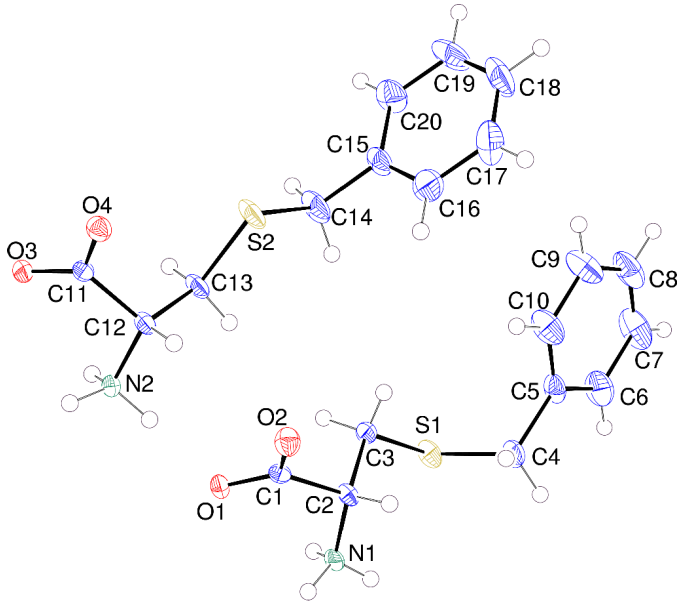


Figure 1
The structure of (I) showing 50% displacement ellipsoids and arbitrary spheres for the H atoms.

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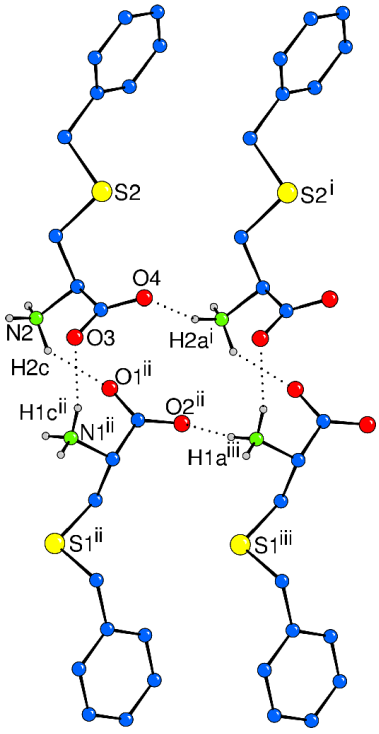

Figure 2
Hydrogen bonding in (I). [Symmetry codes: (i) $x, y-1, z$; (ii) $-x, -\frac{1}{2}+y, -z$; (iii) $1-x, y-\frac{3}{2}, -z$.]

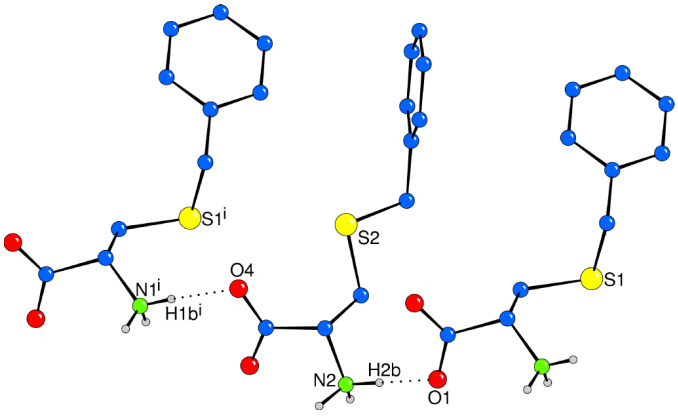

Figure 3
Hydrogen bonding in (I). [Symmetry codes: (i) $x-1, y-1, z$.]

exists in a *gauche* conformation for the N1—C2—C3—S1 grouping, whilst the second (S2) molecule is *anti* about its Cα—Cβ bond (atoms N2—C12—C13—S3). Interestingly, a similar situation occurs for the two asymmetric molecules in monoclinic L-cysteine (Görbitz & Dalhus, 1996). As these authors pointed out, the *gauche* conformation appears to be strongly favoured when cysteine types crystallize. However, in *S*-benzyl-L-cysteinyl-*S*-benzyl-L-cysteine (Capasso *et al.*, 1975), in which two *S*-benzyl-L-cysteine moieties have condensed together, one Cα—Cβ bond is approximately *gauche*, the other *anti*. The absolute structure of the title compound (*R* chirality of C2 and C12) is consistent with that assumed for the L-cysteine starting material.

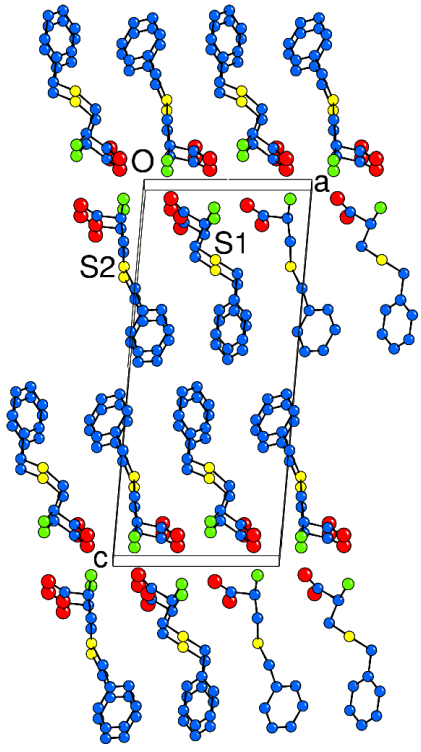

Figure 4
Packing diagram for (I).

Both molecules exist as zwitterions in the crystal. The same situation occurs for monoclinic L-cysteine (Görbitz & Dalhus, 1996). All six N—H entities make hydrogen bonds to nearby carboxyl oxygen species (Table 2 and Figs. 2 and 3) with all four O atoms participating as acceptors, resulting in a two-dimensional network of hydrogen bonds in the (110) plane. As a result, the molecules pack head-to-head (Fig. 4) in a double-sheet structure similar to that seen for other hydrophobic amino acid derivatives (Görbitz & Dalhus, 1996). Unlike the situation in monoclinic L-cysteine, there are no significant S···S contacts [minimum S1···S2 separation in (I) = 4.450 (2) Å], nor are π-stacking interactions involved in defining the structure of the title compound.

Experimental

The title compound was prepared from L-cysteine and benzyl chloride according to the method of Frankel *et al.* (1960). Soft poor quality needles of (I) were recrystallized from hot water.

Crystal data

$C_{10}H_{13}NO_2S$
$M_r = 211.28$
Monoclinic, $P2_1$
$a = 9.4224$ (2) Å
$b = 5.0947$ (1) Å
$c = 21.5510$ (7) Å
$\beta = 94.8950$ (9)°
$V = 1030.77$ (4) Å^3
$Z = 4$
$D_x = 1.361$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 18971 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.29$ mm^{-1}
$T = 293$ (2) K
Rod, colourless
0.10 × 0.05 × 0.04 mm

Data collection

Enraf–Nonius KappaCCD diffractometer	3425 reflections with $I > 2\sigma(I)$
Combination of ω and φ scans	$R_{int} = 0.159$
Absorption correction: multi-scan (*SORTAV*; Nonius, 1999)	$\theta_{max} = 27.5°$
$T_{min} = 0.987$, $T_{max} = 0.989$	$h = -12 \rightarrow 10$
12 824 measured reflections	$k = -6 \rightarrow 6$
4668 independent reflections	$l = -28 \rightarrow 27$
	Intensity decay: none

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} < 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.062$	$\Delta\rho_{max} = 0.42$ e Å^{-3}
$wR(F^2) = 0.160$	$\Delta\rho_{min} = -0.54$ e Å^{-3}
$S = 0.99$	Extinction correction: *SHELXL*97
4668 reflections	Extinction coefficient: 0.011 (4)
254 parameters	Absolute structure: Flack (1983)
H-atom parameters constrained	Flack parameter = −0.19 (10)
$w = 1/[\sigma^2(F_o^2) + (0.0732P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	

Table 1
Selected geometric parameters (Å, °).

S1—C3	1.810 (3)	S2—C13	1.805 (4)
S1—C4	1.834 (4)	S2—C14	1.825 (4)
O1—C1	1.268 (4)	O3—C11	1.258 (4)
O2—C1	1.230 (4)	O4—C11	1.256 (4)
N1—C2	1.486 (4)	N2—C12	1.496 (4)
C1—C2	1.536 (4)	C11—C12	1.528 (5)
C2—C3	1.532 (5)	C12—C13	1.528 (5)
C4—C5	1.510 (5)	C14—C15	1.508 (5)
C3—S1—C4	103.04 (18)	C13—S2—C14	97.86 (17)
O2—C1—O1	126.0 (3)	O4—C11—O3	126.3 (3)
O2—C1—C2	118.1 (3)	O4—C11—C12	116.4 (3)
O1—C1—C2	115.8 (3)	O3—C11—C12	117.3 (3)
N1—C2—C3	109.8 (3)	N2—C12—C13	106.7 (3)
N1—C2—C1	110.6 (3)	N2—C12—C11	109.6 (3)
C3—C2—C1	108.1 (3)	C13—C12—C11	113.6 (3)
C2—C3—S1	114.6 (2)	C12—C13—S2	112.6 (3)
C5—C4—S1	112.5 (3)	C15—C14—S2	109.4 (3)
C1—C2—C3—S1	−168.9 (2)	C11—C12—C13—S2	65.5 (3)
C3—S1—C4—C5	−103.1 (3)	C13—S2—C14—C15	−167.3 (3)
N1—C2—C3—S1	−48.2 (3)	N2—C12—C13—S2	−173.7 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.90	1.96	2.841 (4)	167
N1—H1C···O4^{ii}	0.90	1.91	2.800 (3)	167
N1—H1B···O3^{iii}	0.90	1.96	2.827 (3)	162
N2—H2A···O4^{i}	0.90	1.95	2.832 (4)	168
N2—H2C···O1	0.90	1.84	2.729 (4)	168
N2—H2B···O1^{iv}	0.90	2.07	2.815 (4)	140
N2—H2B···O2^{iii}	0.90	2.43	3.066 (4)	128

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

Data collection: *KappaCCD Software* (Nonius, 1999); cell refinement: *KappaCCD Software*; data reduction: *KappaCCD Software*; 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); software used to prepare material for publication: *SHELXL*97.

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