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N,*N'*-bis(*tert*-butoxycarbonyl)cystamine

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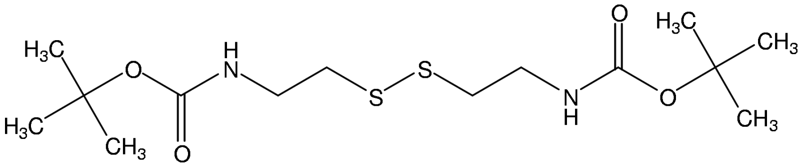
The title compound, Di-Boc-cystamine, $C_{14}H_{28}N_2O_4S_2$, serves as a building block for the synthesis of peptides. The molecule is located on a twofold rotation axis running through the centre of the S—S bond. The crystal packing is stabilized by N—H···O hydrogen bonds.

Key indicators
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.093
Data-to-parameter ratio = 20.5

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

Comment

The title compound, (I), serves as a building block for the synthesis of thioethyl-modified peptides (Moree *et al.*, 1993). The molecule (Fig. 1) possesses C_2 symmetry, with a twofold rotation axis running through the centre of the S—S bond. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 1.6 plus three updates; *MOGUL* Version 1.0; Allen, 2002). The crystal packing (Fig. 2) shows a ladder-like structure in which adjacent molecules are held together by N—H···O hydrogen bonds.



(I)

Experimental

The title compound, (I), was synthesized according to the procedure described by Moree *et al.* (1993). Colourless crystals were grown form an ethanol solution.

Crystal data

$C_{14}H_{28}N_2O_4S_2$
M_r = 352.50
Monoclinic, *C*2/*c*
a = 19.674 (2) Å
b = 9.6968 (8) Å
c = 9.8462 (9) Å
β = 92.589 (5)°
V = 1876.5 (3) Å^3
Z = 4
D_x = 1.248 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 510 reflections
θ = 3.1–19.7°
μ = 0.30 mm^{-1}
T = 173 (2) K
Needle, colourless
0.45 × 0.06 × 0.04 mm

Data collection

Siemens SMART CCD three-circle diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.877, T_{max} = 0.988
7862 measured reflections
2127 independent reflections
1271 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 28.3°
h = −26 → 24
k = −12 → 12
l = −13 → 12

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.093$
$S = 1.02$
2127 reflections
104 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2 + 0.5998P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C2	1.809 (2)	C5—O51	1.220 (2)
S1—S1^i	2.0448 (11)	C5—O6	1.348 (2)
C3—N4	1.449 (3)	O6—C7	1.475 (2)
N4—C5	1.343 (3)		
C2—S1—S1^i	103.12 (7)	O51—C5—O6	125.6 (2)
C3—C2—S1	114.38 (15)	N4—C5—O6	110.54 (18)
C5—N4—C3	120.93 (19)	C5—O6—C7	120.56 (16)
O51—C5—N4	123.9 (2)		
C2^i—S1^i—S1—C2	65.13 (16)		

Symmetry code: (i) $1 - x, y, \frac{1}{2} - z$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N4—H4$\cdots$O51^{ii}	0.79 (2)	2.14 (2)	2.866 (2)	152 (2)

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

H atoms bonded to C atoms were refined with fixed individual displacement parameters [$U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C$_{\rm methylene}$) or 1.5$U_{\rm eq}$(C$_{\rm methyl}$)], using a riding model, with C—H = 0.99 and 0.98 Å, for methylene and methyl H atoms, respectively. The H atom bonded to nitrogen was refined isotropically.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

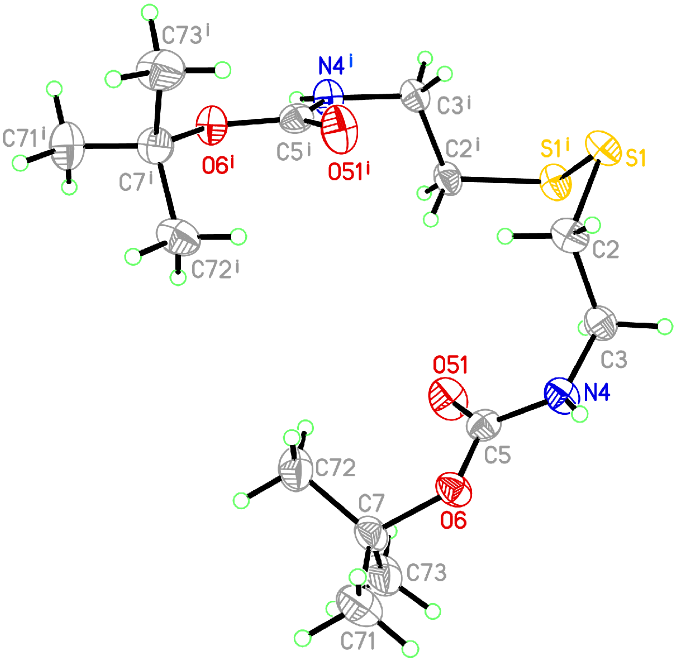

Figure 1
Perspective view of (I), with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level. Symmetry code (i) as in Table 1.

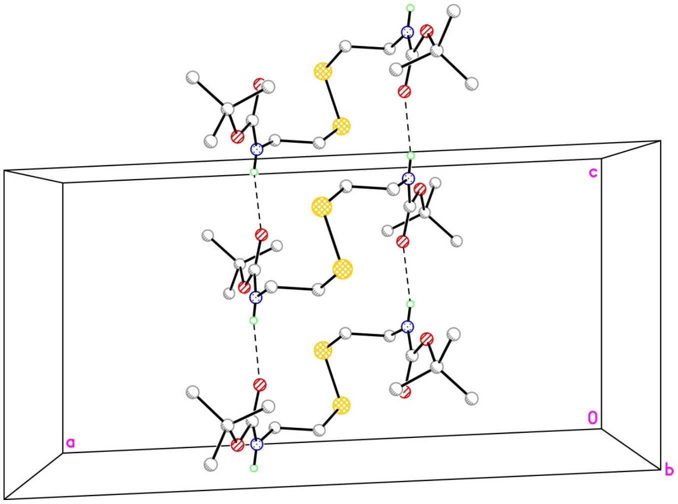

Figure 2
Packing diagram of (I), viewed on the *ac* plane. Hydrogen bonds are shown as dashed lines.

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