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β-DL-Methionine at 105 K

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Key indicators

Single-crystal X-ray study
T = 105 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.100
Data-to-parameter ratio = 17.5

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

In the title compound, $C_5H_{11}NO_2S$, the conformation of the terminal methyl C atom with respect to the β-C atom is *trans*. The crystal structure is stabilized by a network of characteristic head-to-tail DL1 and DL2 sequences.

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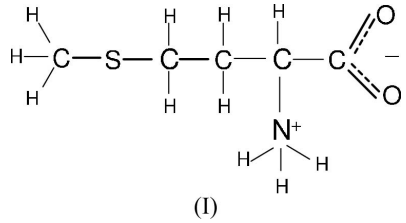
Comment

Methionine, (I), an essential amino acid, is also a principal source of sulfur, which is required by the body for normal metabolism and growth. Previous work on DL-methionine reported the crystal structures of the α- and β-forms (α-DLM1 and β-DLM1) in the space groups $P2_1/a$ (R = 0.21) and $I2/a$ (R = 0.22), respectively, using two-dimensional X-ray intensity data (Mathieson, 1952). Subsequently, redetermination of the crystal structures of the α- and β- forms (α-DLM2 and β-DLM2) was carried out with a view to improving their precision, using three-dimensional X-ray intensity data (R = 0.118 and 0.088, respectively; Taniguchi *et al.*, 1980). The present study (β-DLM3) reports the redetermination of the crystal structure of β-DL-methionine at 105 K.



(I)

Fig. 1 shows the molecular structure of (I), with the atom-numbering scheme. The molecule exists as a zwitterion. The bond lengths and angles are essentially the same as those observed in the earlier studies. The conformation of C5 with respect to C3 is *trans*, as observed in β-DLM2. However, the value of χ_3 [C3—C4—S1—C5] is 174.99 (15)°, somewhat less than the value observed in β-DLM2 (185.6°). In α-DLM2, the terminal C5 atom adopts a gauche conformation, with χ_3 =

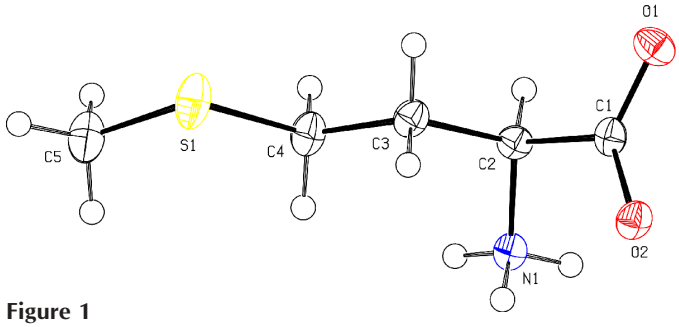


Figure 1
The molecular structure of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids.

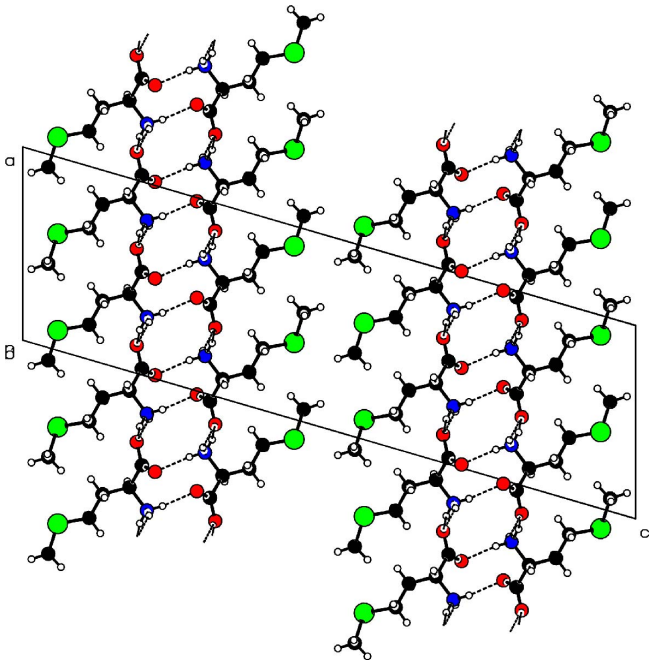


Figure 2
A packing diagram of the molecules of (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

68.9°. Atoms C1, C2, C3, C4 and S form an almost-planar zigzag chain. The torsion angle for the main-chain C atoms (C1—C2—C3—C4) is 173.58 (16)°; this differs somewhat from the value observed in β-DLM2 [185.6°]

Fig. 2 shows the packing of the molecules of (I), viewed along the *b* axis. The mode of aggregation of amino acids and the geometry of the hydrogen-bonding network remain essentially the same as those described for β-DLM2. The crystal structure of (I) is stabilized by a network of characteristic head-to-tail DL1 and DL2 sequences (Vijayan, 1988). These sequences are characterized by interactions between glide-related molecules, with atoms O1 and O2 of the carboxylate group as acceptors. The crystal packing may be visualized as hydrogen-bonded double layers, a characteristic feature of α-amino acids having hydrocarbon side chains, stacked in such a way that the hydrophobic side chains of the methionine molecules are flanked on either side. These double layers extend parallel to the *bc* plane and have only van der Waals interactions between them.

Experimental

Colourless single crystals of (I) were grown as transparent plates by slow evaporation of a saturated aqueous solution.

Crystal data

$C_5H_{11}NO_2S$
M_r = 149.21
Monoclinic, *I*2/*a*
a = 9.877 (2) Å
b = 4.6915 (10) Å
c = 32.603 (6) Å
β = 106.25 (1)°
V = 1450.4 (5) Å^3
Z = 8
D_x = 1.367 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 1012 reflections
θ = 2.6–26.1°
μ = 0.38 mm^{-1}
T = 105 (2) K
Block, colourless
0.32 × 0.24 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.85, T_{max} = 0.92
6469 measured reflections
1436 independent reflections
1373 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.3°
h = −12 → 12
k = −5 → 5
l = −40 → 40

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.100
S = 1.23
1436 reflections
82 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 3.0328P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C5	1.806 (2)	N1—C2	1.483 (2)
S1—C4	1.811 (2)	C1—C2	1.539 (3)
O1—C1	1.261 (2)	C2—C3	1.538 (3)
O2—C1	1.245 (2)	C3—C4	1.536 (3)
C5—S1—C4	100.30 (10)	N1—C2—C1	108.62 (15)
O2—C1—O1	125.64 (18)	C3—C2—C1	109.29 (15)
O2—C1—C2	117.20 (16)	C4—C3—C2	114.56 (16)
O1—C1—C2	117.06 (17)	C3—C4—S1	109.79 (14)
N1—C2—C3	110.07 (15)		
O2—C1—C2—N1	32.6 (2)	N1—C2—C3—C4	54.4 (2)
O1—C1—C2—N1	−150.95 (16)	C1—C2—C3—C4	173.58 (16)
O2—C1—C2—C3	−87.6 (2)	C2—C3—C4—S1	179.23 (13)
O1—C1—C2—C3	88.9 (2)	C5—S1—C4—C3	174.99 (15)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.89	1.93	2.788 (2)	162
N1—H1*B*···O1^{ii}	0.89	2.02	2.814 (2)	148
N1—H1*C*···O1^{iii}	0.89	2.02	2.794 (2)	144

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

All H atoms were positioned geometrically and were allowed to ride on their parent atoms, with C—H = 0.96–0.98 Å and N—H = 0.89 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(N).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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