

**Table 1****Crystal data and structure refinement details for racemic-D-methionyl-D-methionine**

Identification code	racemic-D-methionyl-D-methionine
Sample	Single crystal
Empirical formula	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>
Formula weight	280.40
Temperature/K	149.95(10)
Crystal system	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>a</i> /Å	5.33170(10)
<i>b</i> /Å	20.4441(2)
<i>c</i> /Å	12.34640(10)
$\alpha$ /°	90
$\beta$ /°	95.5590(10)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	1339.45(3)
<i>Z</i> , <i>Z'</i>	4, 1
$\rho_{\text{calc}}$ g/cm <sup>3</sup>	1.390
$\mu$ /mm <sup>-1</sup>	3.616
<i>F</i> (000)	600.0
Crystal size/mm <sup>3</sup>	0.07 × 0.07 × 0.03
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54184)
2 $\Theta$ range for data collection/°	8.396 to 140.524
Index ranges	-6 ≤ <i>h</i> ≤ 6, -24 ≤ <i>k</i> ≤ 24, -15 ≤ <i>l</i> ≤ 15
Reflections collected	14958
Independent reflections	2536 [ <i>R</i> <sub>int</sub> = 0.0379, <i>R</i> <sub>sigma</sub> = 0.0209]
Data/restraints/parameters	2536/0/172
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.046
Final <i>R</i> indexes [ <i>I</i> ≥ 2σ ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.0260, <i>wR</i> <sub>2</sub> = 0.0699
Final <i>R</i> indexes [all data]	<i>R</i> <sub>1</sub> = 0.0283, <i>wR</i> <sub>2</sub> = 0.0727
Largest diff. peak/hole / e Å <sup>-3</sup>	0.32/-0.27
CCDC deposition number	2004931

**Table 2****Crystal data and structure refinement details for racemic-D-methionyl-L-methionine**

Identification code	racemic-D-methionyl-L-methionine
Sample	Powder
Empirical formula	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>
Formula weight	280.40
Temperature/K	293
Crystal system	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>a</i> /Å	16.5974(3)
<i>b</i> /Å	5.3147(1)
<i>c</i> /Å	16.0288(3)
$\alpha$ /°	90
$\beta$ /°	109.3409(13)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	1334.11(5)
Zero point/°	0.0038(4)
<i>Z</i> , <i>Z'</i>	4, 1
$\rho_{\text{calc}}$ g/cm <sup>3</sup>	1.396
2 $\theta$ range/°	4-60
No. of unique reflections	396
No. of parameters	42
<i>R</i> factors	<i>R</i> <sub>wp</sub> (Pawley) = 1.83% <i>R</i> <sub>wp</sub> (Rietveld) = 3.74%
CCDC deposition number	2004932