L-2-aminobutyric acid: two fully ordered polymorphs with *Z*' = 4

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Supplementary material

1. Table 1S. Hydrogen bonding parameters for L-Abu, β-form.

2. Fig. 1S. The asymmetric unit of L-Abu (β-form) with atomic numbering indicated. Thermal ellipsoids have been drawn at the 50% probability level, H-atoms are shown as spheres of arbitrary size.

3. Fig. 2S. (a) The L-Abu $P2_1$ unit cell viewed along the *c*-axis. Only a single layer of A and B molecules is shown. Pseudo *C*-centering is evident.

4. Fig. 3S. Packing of side chains in the structures of (a) L-Abu (α-form), (b) monoclinic L-Cys (Dalhus & Görbitz, 1996) and (c) triclinic L-Val (Flaig *et al*., 2002) in space-fill representation. A weak S-H···S hydrogen bond between Cys side chains is readily detected.

5. Fig. 4S. PXRD patterns for the (a) the α-form and (b) the β-form as calculated by Mercury (Macrae *et al.*, 2008).

References

Dalhus, B. & Görbitz, C. H. (1996). *Acta Chem. Scand*. **50**, 544-548.

Flaig, R., Koritsanszky, T., Dittrich, B., Wagner, A. & Luger, P. (2002). *J. Am. Chem. Soc.* **124**, 3407-3417.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.*, **41**, 466-470.

Table 1S

Hydrogen bond distances (Å) and angles (°) for L-Abu (β-form). The N-H distances were fixed to 0.91 Å.

Bond	H···O	N···O	N-H···O
N1A-H1A···O1B^{i}	1.89	2.775(4)	162
N1A-H2A···O1B^{ii}	1.94	2.816(4)	160
N1A-H3A···O2A^{ii}	1.87	2.769(4)	168
N1B-H1B···O1A^{iii}	1.91	2.798(4)	163
N1B-H2B···O1A^{iv}	1.92	2.799(3)	163
N1B-H3B···O2B^{ii}	1.87	2.773(4)	173
N1C-H1C···O1D^{v}	1.98	2.824(4)	154
N1C-H2C···O2C^{vi}	1.92	2.804(4)	164
N1C-H3C···O1D^{vi}	1.94	2.821(4)	163
N1D-H1D···O1C^{vii}	1.91	2.780(4)	160
N1D-H2D···O2D^{vi}	1.87	2.756(4)	164
N1D-H3D···O1C^{iv}	1.95	2.817(4)	159

Symmetry codes: (i) –x, y, –z, (ii) x, y + 1, z, (iii) 1 – x, y, –z, (iv) x + 1, y, z, (v) ½ – x, y – ½, ½ – z, (vi) x, y – 1, z, (vii) ½ – x, y + ½, ½ – z.

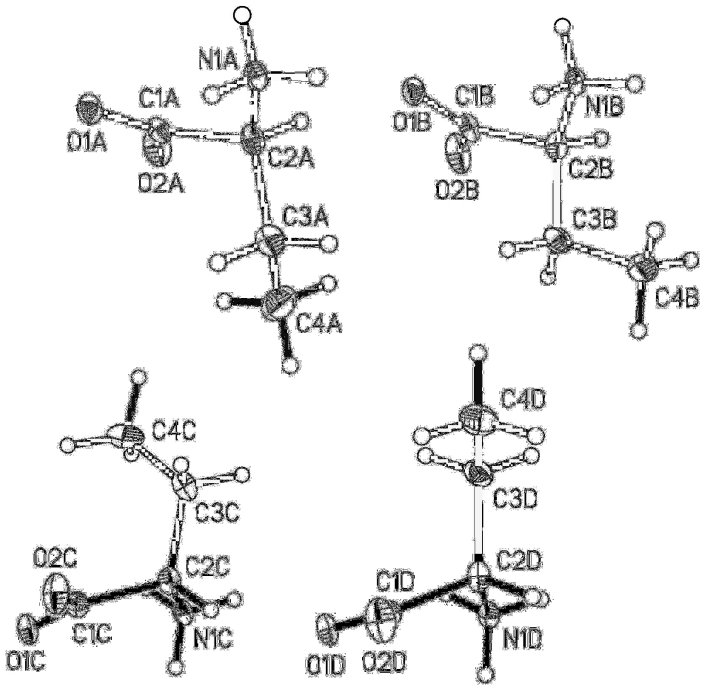


Fig. 1S

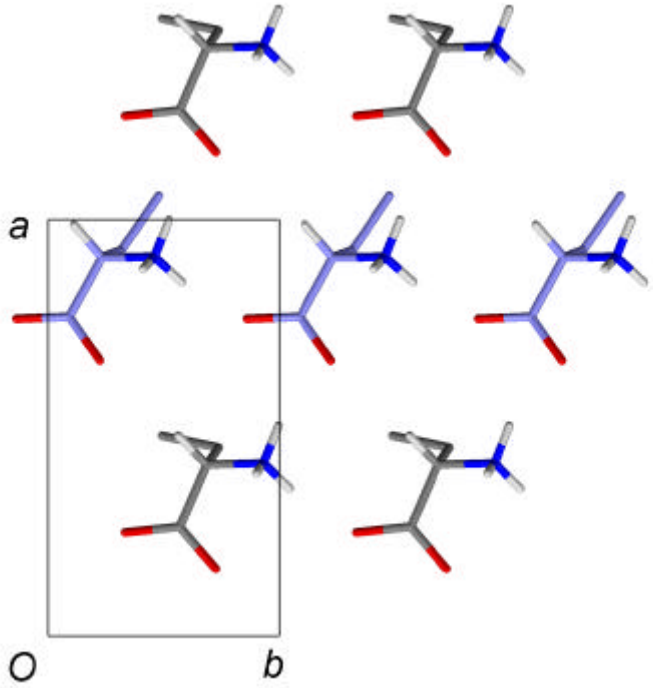
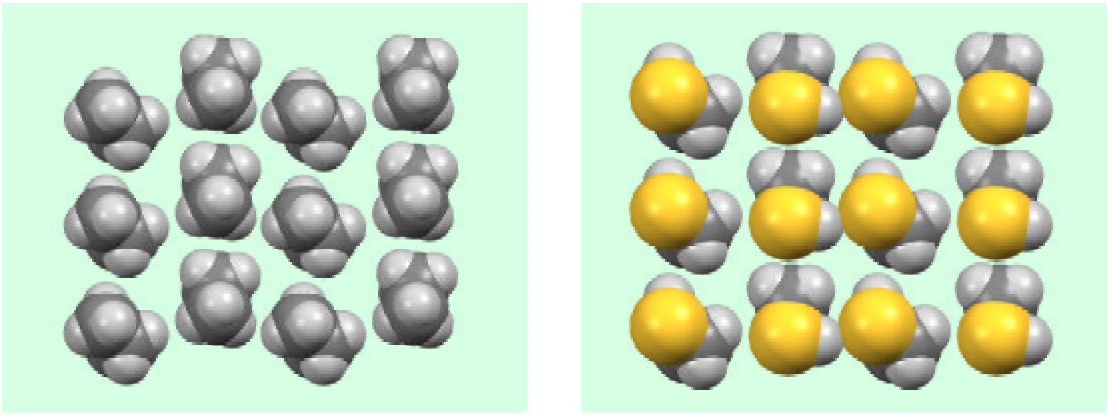


Fig. 2S



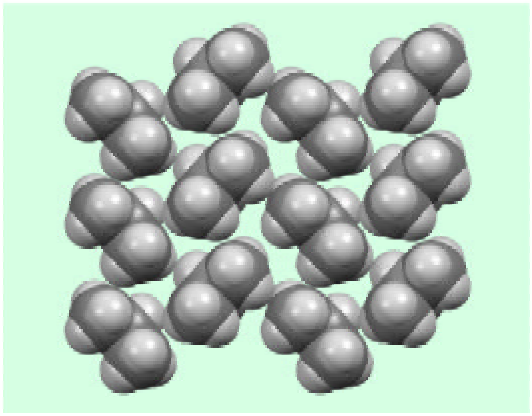
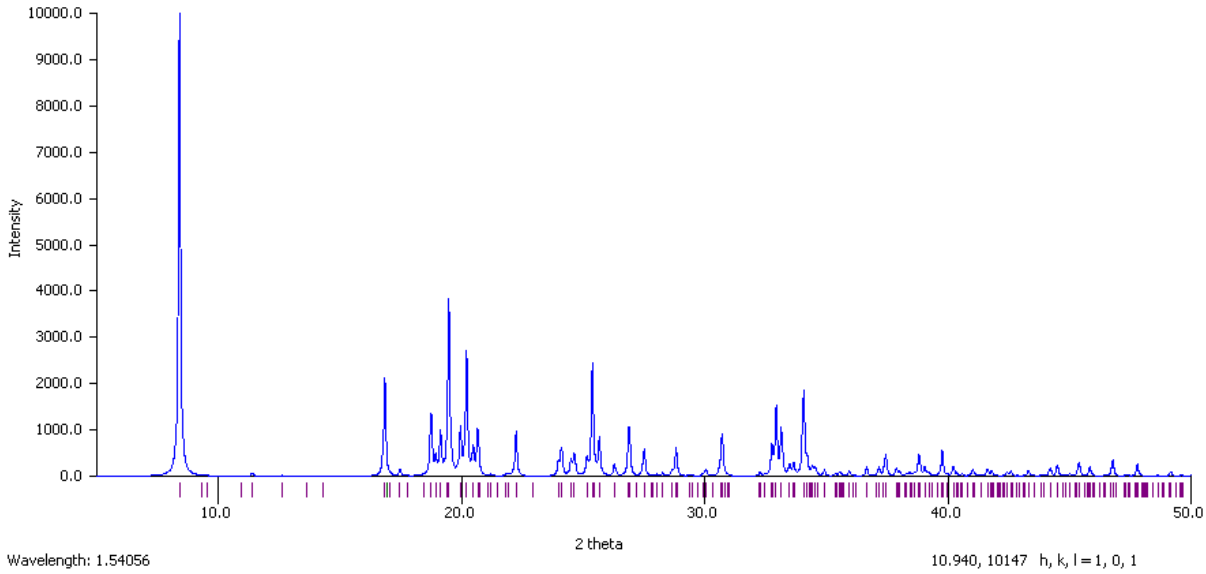


Fig. 3S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6000.0
5000.0
4000.0
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0.0
Intensity
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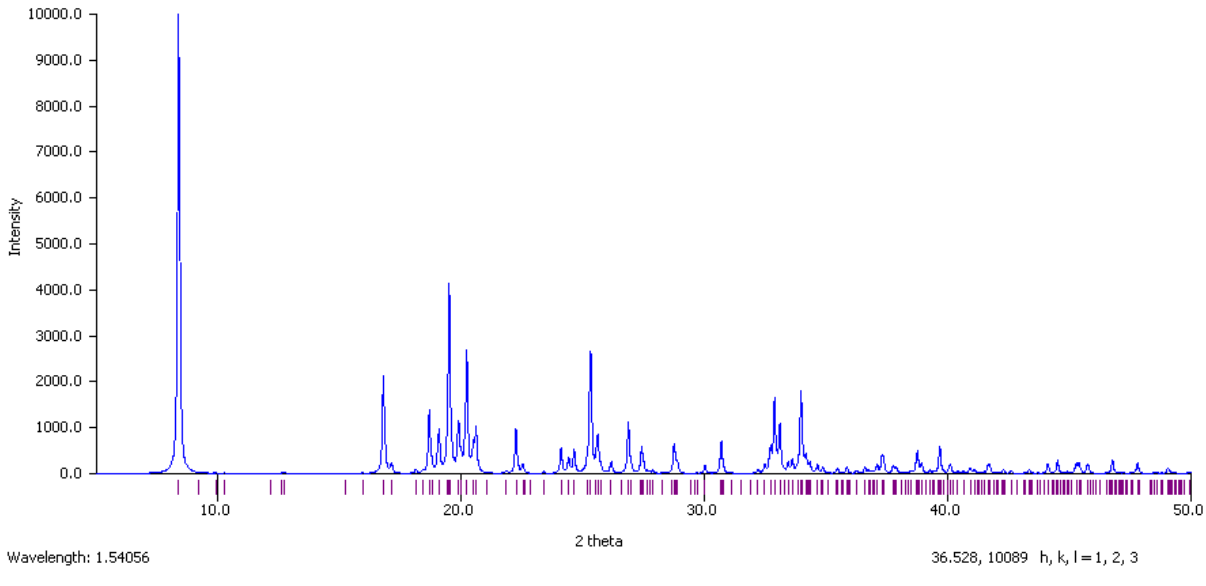
20.0
30.0
40.0
50.0
2 theta
Wavelength: 1.54056
10.940, 10147 h, k, l = 1, 0, 1

(a)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0.0
Intensity
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20.0
30.0
40.0
50.0
2 theta
Wavelength: 1.54056
36.528, 10089 h, k, l = 1, 2, 3

(b)

Fig. 4S