of these observations. Alternatively, consideration of the benzene rings alone would again suggest that it be described in terms of individually planar but not coplanar salicylaldimine groups, separated by 0·2 Å. The experimental accuracy is not sufficient to distinguish a planar molecule from one that is slightly stepped. These variations between *A* and *B* must presumable stem from packing effects, and would support the contention (Cheeseman, Hall & Waters, 1965) that the resistance of such molecules to deformation from overall planarity is rather less than has often been supposed.

The coordination is square planar, the closest contacts made by the copper atoms in the octahedral axial direction being in each case to atoms C(8) of adjacent molecules along [010], and of length 3·37 and 3·39 Å for molecules *A* and *B* respectively. The molecules are so oriented that the ethanolic hydroxyl groups of the independent molecules make contacts of 2·65 and 2·70 Å. The structure may then be described in terms of two-dimensional sheets of hydrogen-bonded molecules, parallel to (001). The compactness of this structure, resulting from the hydrogen bond formation, may be seen by comparing the density, 1·495 g.cm^{-3}, with the values of 1·405 for bis-(*N*-ethylsalicylaldiminato)-copper (Clark, 1964) and 1·34 for bis-(*N*-butylsalicylaldiminato)copper (calculated from Frasson *et al.*, 1964).

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Refinement of the L-alanine crystal structure.

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Shortly after we had completed the measurement of a set of three-dimensional intensities for a crystal of L-alanine, we learned that the crystal structure had recently been determined by Simpson & Marsh (1966). In order to test the constancy of the molecular parameters derived from different data sources, we have carried out a series of full-matrix least-squares refinements with our data. We present here the comparison of our results with those of Simpson & Marsh (SM).

Our intensity measurements were made with a Hilger–Watts linear diffractometer, using Mo radiation with SrO/ZrO$_2$ balanced filters. The intensities of 522 independent reflexions were recorded in the layers *hk*0 – *hk*6 and converted to relative *F* values in the usual way. Absorption corrections were not deemed necessary.

Starting with SM's published parameters for the C, N and O atoms (hydrogen atoms were included in the structure factor calculations but not refined), our analysis leads to the results shown in Tables 1 and 2. The agreement is good as far as the chemical significance of the results is concerned; however, the differences, although small, seem statistically significant on the basis of the estimated standard deviations cited by SM. (We have not calculated the least-squares standard deviations of our parameters, but they should be of about the same order of magnitude as those of SM.) On the basis of tests using the function $R'' = [\sum_i w_i(F_o-F_c)^2/\sum_i w_iF_o^2]^{\frac{1}{2}}$ (Hamilton, 1965) we find that our data reject the SM model at better than 0·005 level of significance, while the SM data reject our model at about the same level.

Table 1. *Positional parameters* (× 10^4) *and bond lengths*

	x_{DR}	x_{SM}	σ_{SM}	y_{DR}	y_{SM}	σ_{SM}	z_{DR}	z_{SM}	σ_{SM}
O(1)	7278	7287	3	843	843	1	6280	6283	3
O(2)	4499	4501	3	1856	1850	1	7604	7609	3
C(1)	5606	5606	4	1413	1418	1	6023	6016	4
N	6565	6560	3	1375	1382	1	1853	1856	3
C(2)	4764	4769	4	1611	1612	1	3559	3563	4
C(3)	2744	2746	5	919	915	2	3021	3025	5

Bond	d_{DR}	d_{SM}
C(1)–O(1)	1·239 Å	1·247 Å
C(1)–O(2)	1·257	1·256
C(1)–C(2)	1·533	1·525
C(2)–C(3)	1·523	1·525
C(2)–N	1·496	1·491

$$\frac{R''\ (\text{SM data: our model})}{R''\ (\text{SM data: SM model})} = \frac{0{\cdot}091}{0{\cdot}070} = 1{\cdot}30$$

$$\frac{R''\ (\text{our data: SM model})}{R''\ (\text{our data: our model})} = \frac{0{\cdot}066}{0{\cdot}049} = 1{\cdot}34\,.$$

Table 2. *Anisotropic temperature factors* (× 10⁴)

		b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
O(1)	DR	217	46	177	62	−67	21
	SM	206	44	151	59	−47	16
	σSM	6	1	6	4	10	4
O(2)	DR	233	52	118	44	25	−10
	SM	227	53	91	46	18	−10
	σSM	7	1	5	4	10	3
C(1)	DR	169	27	142	6	−59	12
	SM	149	25	119	−6	−18	−8
	σSM	6	1	7	4	10	4
N	DR	176	41	99	14	−13	−3
	SM	150	36	88	5	12	2
	σSM	6	1	6	4	8	4
C(2)	DR	163	36	121	42	−8	−1
	SM	138	28	98	15	5	−4
	σSM	6	1	7	4	10	4
C(3)	DR	195	62	163	−26	−35	−2
	SM	177	58	153	−38	−61	−15
	σSM	8	2	9	5	12	5

The goodness of fit for both sets of data to their corresponding models is about the same; for our data $R=0{\cdot}061$, $R''=0{\cdot}049$, for the SM data $R=0{\cdot}049$, $R''=0{\cdot}070$, with R'' based on the 489 reflexions common to both data sets ($R=\sum_i |F_o-F_c|/\sum_i |F_o|$). We conclude that the small differences between our model and that of SM arise mainly from systematic errors in the data.

In carrying out the Hamilton tests, weights for the SM data were estimated from SM's expression for $\sigma(F_o^2)$ using $\sigma(F_o)\sim\sigma(F_o^2)/2F_o$. For our data, and also in the latter stages of our refinement, we employed a weighting system $w_i=64/F_o^2, F_o\geq 8$; $w_i=F_o^2/64, F_o\leq 8$, which was found empirically to give a reasonably constant value of $\sum_i w_i(F_o-F_c)^2/n$ in different ranges of F_o. Some earlier calculations were carried out with weights based on the estimated intensity errors arising solely from statistical counting fluctuations. Since the diffractometer operates on a fixed-time counting mode, weak reflexions are here assigned in general low weights, while strong reflexions are assigned a high and more or less constant weight. The unsuitability of this weighting scheme soon became apparent from the $\sum_i w_i(F_o-F_c)^2/n$ test, but it is interesting that it led to large errors not only in the thermal parameters but also in the positions of the atoms. The change in the position of C(3) amounted to 0·035 Å, about ten times the estimated standard deviation, with a concomitant change in the C(2)–C(3) bond length from 1·525 Å (SM) to 1·553 Å!! This impresses the importance to be attached to a suitable weighting system for least-squares refinement.

We are grateful to Dr R.E. Marsh for making his L-alanine data available to us prior to publication.

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A program to contour Fourier maps by use of an incremental CRT display.

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A method of automatically contouring Fourier syntheses by use of the on-line incremental CRT display type 340 has been developed as one of a series of programs written for the University of Western Australia's PDP 6 computer. The display unit operates on a network of 1024 × 1024 points which occupy a screen area of 10″ × 10″. The two principal modes of operation are (i) *the point mode* where the coordinates of an individual point are stored in a 36-bit word and (ii) *the vector mode* where the components of a vector are stored in an 18-bit half-word. The vector mode can also be used to increment the display coordinates without intensifying the screen. The time required to display a point is 30 μ sec, while a vector is drawn at a speed corresponding to 1·5 μ sec per point.

A method of plotting syntheses on a point by point principle has been developed for an X–Y plotter by Cherin, Madigan & Martin (1965). It would be possible to apply this technique directly to the CRT display. However, the figures given above show that the display is much more efficient with regard to both speed and storage required when used in the vector mode. The present method was therefore developed so as to utilize this feature as much as possible.

The details of the calculation are best understood by reference to Fig. 1. This represents a grid unit $ABCD$ with electron density values of 30, 20, 60 and 10 at the corners. It is assumed that contours are required at 25 and 50 with the first level broken. A linear interpolation is performed along AB to obtain the coordinates of the point P where the electron density has the value 25. Points Q, R and S are similarly located. To resolve the ambiguity as to whether the contours at $\varrho=25$ are along PS and RQ or RS and PQ, the function $|\varrho_A+\varrho_C-25|-|\varrho_B+\varrho_D-25|$ is examined. In this example the function is positive, so the contours are taken to be RS and PQ. Vectors are then set up as follows.

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