

X-ray experimental details

Datasets were collected on a Bruker diffractometer at the indicated temperature using MoK α radiation. Data were collected using SMART^(a) or APEXII software.^(b) Initial cell constants were found by small widely separated “matrix” runs. An entire hemisphere of reciprocal space was collected. Scan speed and scan width were chosen based on scattering power and peak rocking curves.

Unit cell constants and orientation matrix were improved by least-squares refinement of reflections thresholded from the entire dataset. Integration was performed with SAINT,^(c) using this improved unit cell as a starting point. Precise unit cell constants were calculated in SAINT from the final merged dataset. Lorenz and polarization corrections were applied. Except where noted, absorption corrections were not applied.

Data were reduced with SHELXTL.^(d) The structures were solved in all cases by direct methods without incident. Where possible, the coordinates of the amide hydrogen atoms were refined. All other hydrogen atoms were assigned to idealized positions and were allowed to ride. All molecules were fully ordered and no solvent was present in any of the samples.

7 Coordinates for the amide protons H17A & H17B were allowed to refine.

8 Coordinates for the amide protons H17A & H17B were allowed to refine.

9 Coordinates for the amide protons H27A & H27B were allowed to refine. Atoms C15 and C17 were unstable to anisotropic refinement and were given isotropic thermal parameters.

10 Coordinates for the amide protons H27A & H27B were allowed to refine. Data were corrected for absorption.

11 Coordinates for the amide protons H17A & H17B were allowed to refine.

12 The compound crystallized with two independent molecules per asymmetric unit. Data were corrected for absorption. Amide protons H27A & H27B and H47A & H47B were placed in idealized positions and were allowed to ride.

(a) SMART v5.060, © 1997 - 1999, Bruker Analytical X-ray Systems, Madison, WI.

(b) APEXII v1.27, © 2005, Bruker Analytical X-ray Systems, Madison, WI.

(c) SAINT v6.02, © 1997 - 1999, Bruker Analytical X-ray Systems, Madison, WI.

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(d) SHELXTL v5.10, © 1997, , Bruker Analytical X-ray Systems, Madison, WI.