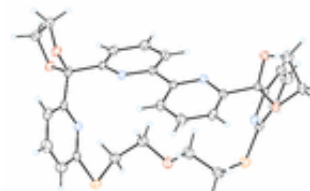


Summary report for Directory: home/fronz/data/SOSMacro

Report generated Apr 04, 2011; 16:05:36

Unit cell

8098 reflections with $2.55^\circ < \theta < 30.03^\circ$ (resolution between 8.00Å and 0.71Å) were used for unit cell refinement



Symmetry used in scalepack	p2
a (Angstrom)	13.4189 +/- 0.0003
b (Angstrom)	13.7584 +/- 0.0003
c (Angstrom)	16.1094 +/- 0.0003
alpha (°)	90.000
beta (°)	106.2590 +/- 0.0015
gamma (°)	90.000
Volume (Å**3)	2855.21 +/- 0.11
Mosaicity (°)	0.5010 +/- 0.0010

Data collection

Summary

Total number of images collected	288
Total exposure time	229.0 minutes
Data collection exposure time	222.3 minutes
Data collection wall-clock time	253.3 minutes

Experimental Conditions

Wavelength	0.71073 Å
Cryostat setting	100.00K
Generator setting	55kV 20mA

Scans

Type	Name	# images	Total Rotation	Per frame Rotation	Exposure per frame	Detector distance	Used in scaling
cell determination	i01f	10	10.0° phi	1.000°	40 seconds	45.00 mm	No
data collection	s01f	133	266.0° phi	2.000°	60 seconds	40.00 mm	Yes
data collection	s02f	64	128.0° omega	2.000°	60 seconds	40.00 mm	Yes
data collection	s03f	81	162.0° phi	2.000°	18 seconds	40.00 mm	Yes

Scalepack Scaling

Deleted observations

Rejected	88
Zero sigma or profile test	3
Overload or incomplete profile	1322
Sigma cutoff	41
High resolution limit	15

Final Data Set

Scale factor range	2.90-10.17
Number of 'full' reflections	27855
Number of 'partial' reflections	14757
Total number of integrated reflections	38312
Total number of unique reflections	8612
Data completeness	99.3%
Resolution range	8.00-0.71 Å
Theta range	2.55°-30.03°
Average Intensity	78.2
Average Sigma(I)	3.0
Overall R-merge (linear)	0.046

[*Bruker AXS Collect software*](#)