

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lili3_ken

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: lili3_ken

Bond precision: C-C = 0.0045 Å Wavelength=1.54178

Cell: a=9.3589(2) b=18.2694(4) c=18.3048(5)
 alpha=78.384(1) beta=79.725(1) gamma=89.882(1)
Temperature: 193 K

	Calculated	Reported
Volume	3014.66(12)	3014.66(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H20 O2 S	C17 H20 O2 S
Sum formula	C17 H20 O2 S	C17 H20 O2 S
Mr	288.39	288.39
Dx, g cm ⁻³	1.271	1.271
Z	8	8
Mu (mm ⁻¹)	1.889	1.889
F000	1232.0	1232.0
F000'	1237.80	
h, k, lmax	11, 22, 22	11, 22, 22
Nref	12382	12203
Tmin, Tmax	0.762, 0.828	0.820, 1.000
Tmin'	0.753	

Correction method= # Reported T Limits: Tmin=0.820 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.986 Theta(max)= 74.729

R(reflections)= 0.0625(8952)	wR2(reflections)=
S = 1.018	0.1889(12203)
Npar= 758	

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.



Alert level C

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00452	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.838	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	47	Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	15%	Note
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1B -C10B .	1.42	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1 -C10 .	1.42	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1C -C10C .	1.42	Ang.
PLAT410_ALERT_2_G	Short Intra H...H Contact H7B ..H13A .	2.02	Ang.
	x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H10B ..H14A .	2.02	Ang.
	x,y,z =	1_555	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C17 H20 O2 S	2	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C17 H20 O2 S	3	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	46	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	132	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.1	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

19 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

10 ALERT type 2 Indicator that the structure model may be wrong or deficient

7 ALERT type 3 Indicator that the structure quality may be low

5 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

