

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bmk1962b

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: bmk1962b

Bond precision: C-C = 0.0042 Å Wavelength=0.71073

Cell: a=9.6162 (6) b=13.2978 (11) c=14.2415 (11)
 alpha=70.629 (7) beta=74.519 (6) gamma=72.199 (7)
Temperature: 293 K

	Calculated	Reported
Volume	1607.8 (2)	1607.8 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H19 N3 O2 S, C17 H16 O3 ?	
Sum formula	C35 H35 N3 O5 S	C35 H35 N3 O5 S
Mr	609.72	609.72
Dx, g cm ⁻³	1.260	1.259
Z	2	2
Mu (mm ⁻¹)	0.146	0.146
F000	644.0	644.0
F000'	644.52	
h, k, lmax	13, 18, 20	13, 18, 17
Nref	9352	7698
Tmin, Tmax	0.982, 0.989	0.727, 1.000
Tmin'	0.945	

Correction method= # Reported T Limits: Tmin=0.727 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.823 Theta(max)= 29.972

R(reflections)= 0.0633 (3716)	wR2(reflections)=
S = 1.028	0.1808 (7698)
Npar= 401	

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 B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 14 Note



Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 48% Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00422 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 8.010 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT793_ALERT_4_G Model has Chirality at C10 (Centro SPGR) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1432 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.0 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 3 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 3 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
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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.

