

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 22kub79_0m_a

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: 22kub79_0m_a

Bond precision:	C-C = 0.0109 Å	Wavelength=0.71073	
Cell:	a=20.821 (6)	b=13.485 (3)	c=9.9001 (17)
	alpha=90	beta=90	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	2779.7 (11)	2779.7 (11)	
Space group	P n a 21	P n a 21	
Hall group	P 2c -2n	P 2c -2n	
Moiety formula	C16 H36 N, C2 H14 B10 N S	C2 H14 B10 N S, C16 H36 N	
Sum formula	C18 H50 B10 N2 S	C18 H50 B10 N2 S	
Mr	434.76	434.76	
Dx, g cm ⁻³	1.039	1.039	
Z	4	4	
Mu (mm ⁻¹)	0.126	0.126	
F000	952.0	952.0	
F000'	952.67		
h, k, lmax	27, 17, 13	27, 17, 12	
Nref	6620 [3500]	6183	
Tmin, Tmax	0.941, 0.975	0.666, 0.746	
Tmin'	0.927		

Correction method= # Reported T Limits: Tmin=0.666 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.77/0.93 Theta (max)= 27.876

R(reflections)= 0.0787 (4843)

wR2(reflections)=
0.2227 (6183)

S = 1.031

Npar= 296

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**

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01092 Ang.

 **Alert level C**

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 8 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 5 Note

 **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C5 --C6B . 6.7 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 6% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 10 Note
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u. 0.04 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 4 Note
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 3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.9 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
1 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
4 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

PLATON version of 10/05/2023; check.def file version of 10/05/2023

