

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_22kub31_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: mo_22kub31_0m_a

Bond precision:	C-C = 0.0040 Å	Wavelength=0.71073	
Cell:	a=13.711(6)	b=17.515(3)	c=17.391(5)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	4176(2)	4177(2)	
Space group	P b c n	P b c n	
Hall group	-P 2n 2ab	-P 2n 2ab	
Moiety formula	C2 H14 B12 N, C8 H20 N	C2 H14 B12 N, 2(C4 H10 N0.5)	
Sum formula	C10 H34 B12 N2	C10 H34 B12 N2	
Mr	312.11	312.11	
Dx, g cm ⁻³	0.993	0.993	
Z	8	8	
Mu (mm ⁻¹)	0.049	0.049	
F000	1344.0	1344.0	
F000'	1344.19		
h,k,lmax	16,21,21	16,21,21	
Nref	4103	4079	
Tmin,Tmax	0.988,0.995	0.586,0.746	
Tmin'	0.976		

Correction method= # Reported T Limits: Tmin=0.586 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.996

R(reflections)= 0.0886(3081)	wR2(reflections)= 0.2738(4079)
S = 1.033	Npar= 223

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

PLAT049_ALERT_1_B	Calculated Density Less Than 1.0 gcm-3	0.9929	Check
PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	0.93	eA-3



Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.27	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.53	Report
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.125	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	17	Report



Alert level G

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.16	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.16	Why ?
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	8	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.1	Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0	Degree
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
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

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

