

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jb250221_1_1

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: jb250221_1_1

Bond precision:	C-C = 0.0058 A	Wavelength=0.71073	
Cell:	a=17.517(13)	b=6.924(5)	c=7.458(6)
	alpha=90	beta=97.957(16)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	895.9(12)	895.9(11)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C7 H6 B F3 K N O2	C7 H6 B F3 K N O2	
Sum formula	C7 H6 B F3 K N O2	C7 H6 B F3 K N O2	
Mr	243.04	243.04	
Dx,g cm-3	1.802	1.802	
Z	4	4	
Mu (mm-1)	0.616	0.616	
F000	488.0	488.0	
F000'	489.15		
h,k,lmax	22,9,9	22,9,9	
Nref	2063	2053	
Tmin,Tmax	0.943,0.988	0.602,0.746	
Tmin'	0.868		

Correction method= # Reported T Limits: Tmin=0.602 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 27.539

R(reflections)= 0.0565(1227) wR2(reflections)= 0.1284(2053)

S = 1.007 Npar= 137

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.11	Report
PLAT213_ALERT_2_C	Atom C2 has ADP max/min Ratio	3.5	oblate
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.2	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0058	Ang.
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.80A From N1	0.41	eA-3



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.18	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #	90	Check
	01 -C1 -K1 1.555 1.555 1.565	42.70	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	30	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	10	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

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

- 0 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
4 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
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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.

