

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 025rlr003

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: 025rlr003

Bond precision:	C-C = 0.0072 A	Wavelength=1.54184	
Cell:	a=5.6891(4)	b=14.7673(5)	c=19.7659(6)
	alpha=90	beta=96.186(4)	gamma=90
Temperature:	150 K		

	Calculated	Reported
Volume	1650.92 (14)	1650.92 (14)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C14 H20 Br K N2 O2	C14 H20 Br K N2 O2
Sum formula	C14 H20 Br K N2 O2	C14 H20 Br K N2 O2
Mr	367.32	367.33
Dx, g cm-3	1.478	1.478
Z	4	4
Mu (mm-1)	5.676	5.676
F000	752.0	752.0
F000'	752.44	
h, k, lmax	7, 18, 24	7, 18, 24
Nref	3471	3427
Tmin, Tmax	0.356, 0.639	0.338, 1.000
Tmin'	0.090	

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Correction method= # Reported T Limits: Tmin=0.338 Tmax=1.000
AbsCorr = MULTI-SCAN
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Data completeness= 0.987 Theta (max)= 76.521

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R(reflections)= 0.0464( 2632)      wR2(reflections)=
S = 1.054                        0.1327( 3427)
Npar= 291
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The following ALERTS were generated. Each ALERT has the format

Click on the hyperlinks for more details of the test.

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	4.0	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	4.6	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq	as Compared to Neighbors of		C12	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq	as Compared to Neighbors of		C13	Check
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds			0.00717	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3)	Bond C11	- C12		1.43	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance				2.056	Check

[illegible]

7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
34 **ALERT level G** = General information/check it is not something unexpected

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

