

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bmk2015b

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: bmk2015b

Bond precision:	C-C = 0.0046 Å	Wavelength=1.54184	
Cell:	a=23.0527(11)	b=11.8887(5)	c=7.2229(3)
	alpha=90	beta=90	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	1979.56(15)	1979.56(15)	
Space group	P c a 21	P c a 21	
Hall group	P 2c -2ac	P 2c -2ac	
Moiety formula	C20 H20 N6 O S	?	
Sum formula	C20 H20 N6 O S	C20 H20 N6 O S	
Mr	392.48	392.48	
Dx, g cm ⁻³	1.317	1.317	
Z	4	4	
Mu (mm ⁻¹)	1.641	1.641	
F000	824.0	824.0	
F000'	827.53		
h, k, lmax	29, 15, 9	28, 14, 9	
Nref	4171 [2260]	3397	
Tmin, Tmax	0.834, 0.929	0.484, 1.000	
Tmin'	0.586		

Correction method= # Reported T Limits: Tmin=0.484 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 1.50/0.81 Theta(max)= 76.778

R(reflections)= 0.0369(3185)	wR2(reflections)= 0.0989(3397)
S = 1.050	Npar= 255

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

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N2	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C11	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C8	Check
PLAT340_ALERT_3_C	Low	Bond Precision on	C-C Bonds	0.00461	Ang.



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT792_ALERT_1_G	Model has Chirality at C12 (Polar 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	5	Note
PLAT915_ALERT_3_G	No Flack x Check Done: Low Friedel Pair Coverage	60	%
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1	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
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 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.

