

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hsy-20241223exp_102_auto

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: hsy-20241223exp_102_auto

Bond precision:	C-C = 0.0020 A	Wavelength=1.54184	
Cell:	a=7.5522 (1)	b=13.2198 (2)	c=14.4340 (2)
	alpha=90	beta=91.968 (1)	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	1440.22 (4)	1440.22 (4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 H13 N O5 S	C16 H13 N O5 S
Sum formula	C16 H13 N O5 S	C16 H13 N O5 S
Mr	331.33	331.33
Dx, g cm-3	1.528	1.528
Z	4	4
Mu (mm-1)	2.252	2.252
F000	688.0	688.0
F000'	691.52	
h, k, lmax	9, 16, 17	9, 16, 17
Nref	2918	2869
Tmin, Tmax	0.467, 0.798	0.154, 1.000
Tmin'	0.353	

Correction method= # Reported T Limits: Tmin=0.154 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.983 Theta (max)= 73.879

```
R(reflections)= 0.0340( 2792)      wR2(reflections)=
S = 1.059                        0.0909( 2869)
Npar= 210
```

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
1 0 0, 1 0 2,



Alert level G

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 30 Note
S01 C008 C009 C00A C00B C00C H00C C00D
C00E H00E C00F H00F C00G H00G C00H H00H
C00I H00I C00J H00J C00K H00K C00L H00L
C00M H00A H00B H00D C00N H00N
PLAT793_ALERT_4_G Model has Chirality at C00C (Centro SpGr) R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 47 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
1 0 2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 5.681 Note
Predicted wR2: Based on SigI**2 1.60 or SHELX Weight 8.59
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 12 Info

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

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
3 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.

