

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) chsu242lt_0m

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: chsu242lt_0m

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=18.877(4) b=16.644(3) c=19.387(4)
 alpha=90 beta=91.781(10) gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	6088(2)	6088(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C15 H13 N O2	C15 H13 N O2
Sum formula	C15 H13 N O2	C15 H13 N O2
Mr	239.26	239.26
Dx,g cm-3	1.305	1.305
Z	20	20
Mu (mm-1)	0.087	0.087
F000	2520.0	2520.0
F000'	2521.15	
h,k,lmax	25,22,25	25,22,25
Nref	15345	15117
Tmin,Tmax	0.996,0.998	0.746,0.746
Tmin'	0.996	

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

Data completeness= 0.985 Theta(max)= 28.439

R(reflections)= 0.0579(8761) wR2(reflections)= 0.1596(15117)

S = 1.025 Npar= 816

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**

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O4C	--	C15C	..	5.7	su
PLAT410_ALERT_2_C	Short Intra H...H Contact	H2A	..	H10A	..	1.97	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H2B	..	H10B	..	1.97	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H2D	..	H10D	..	1.99	Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor	N1C	-	H1CA	..		Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N1A	-	H1AA	..		Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N1E	-	H1EA	..		Please Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance				4.906	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600				7	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF				1	Note
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much smaller I(calc)	.				1	Check

● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms				15	Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				15	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600				224	Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **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
4 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*, 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.

PLATON version of 21/04/2015; check.def file version of 09/03/2015

