checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Hsu_HHS465, Hsu_HHS475, Hsu_HHS483

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: Hsu_HHS465

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Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:           a=10.5551(15)    b=4.8430(7)       c=12.5583(18)
                alpha=90         beta=96.404(3)    gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          637.95(16)                637.95(16)
Space group     P 21                      P 1 21 1
Hall group      P 2yb                     P 2yb
Moiety formula  C12 H10 N4 O3 S           ?
Sum formula     C12 H10 N4 O3 S           C12 H10 N4 O3 S
Mr              290.30                    290.30
Dx,g cm-3       1.511                     1.511
Z               2                         2
Mu (mm-1)       0.267                     0.267
F000            300.0                     300.0
F000'           300.37
h,k,lmax        15,6,17                   15,6,17
Nref            3881[ 2151]               3793
Tmin,Tmax       0.921,0.974               0.900,0.970
Tmin'           0.815

Correction method= # Reported T Limits: Tmin=0.900 Tmax=0.970
AbsCorr = MULTI-SCAN

Data completeness= 1.76/0.98      Theta(max)= 30.520

R(reflections)= 0.0253( 3656)     wR2(reflections)= 0.0652( 3793)

S = 1.066                 Npar= 185
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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 G

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PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       0.77 mm
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         11 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 Check
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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
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

0 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
0 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

Datablock: Hsu_HHS475

Bond precision: C-C = 0.0019 A Wavelength=0.71073

Cell: a=9.6261(12) b=9.3462(11) c=29.655(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2668.0(6)	2668.0(6)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C12 H10 N4 O3 S	?
Sum formula	C12 H10 N4 O3 S	C12 H10 N4 O3 S
Mr	290.30	290.30
Dx,g cm-3	1.446	1.445
Z	8	8
Mu (mm-1)	0.256	0.256
F000	1200.0	1200.0
F000’	1201.49	
h,k,lmax	13,12,40	13,12,40
Nref	3604	3604
Tmin,Tmax	0.853,0.948	0.860,0.950
Tmin’	0.853	

Correction method= # Reported T Limits: Tmin=0.860 Tmax=0.950
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 29.130

R(reflections)= 0.0387(3390) wR2(reflections)= 0.0922(3604)

S = 1.177 Npar= 185

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.572 Check

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Alert level G

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.62 mm
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info

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Datablock: Hsu_HHS483

Bond precision: C-C = 0.0064 A Wavelength=0.71073

Cell:	a=33.819(7)	b=10.587(2)	c=9.6316(18)
	alpha=90	beta=94.564(6)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	3437.6(12)	3437.6(11)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C18 H13 F N4 O3 S	?
Sum formula	C18 H13 F N4 O3 S	C18 H13 F N4 O3 S
Mr	384.38	384.38
Dx,g cm-3	1.485	1.485
Z	8	8
Mu (mm-1)	0.227	0.227
F000	1584.0	1584.0
F000'	1585.74	
h,k,lmax	41,12,11	41,12,11
Nref	3309	3297
Tmin,Tmax	0.927,0.988	0.700,0.990
Tmin'	0.927	

Correction method= # Reported T Limits: Tmin=0.700 Tmax=0.990
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.820

R(reflections)= 0.0713(2466) wR2(reflections)= 0.2032(3297)

S = 1.092 Npar= 248

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

PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00644 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H1 ..O3 .	2.66 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	7.056 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3 Report

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Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	24.81 Why ?
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	6 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info

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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

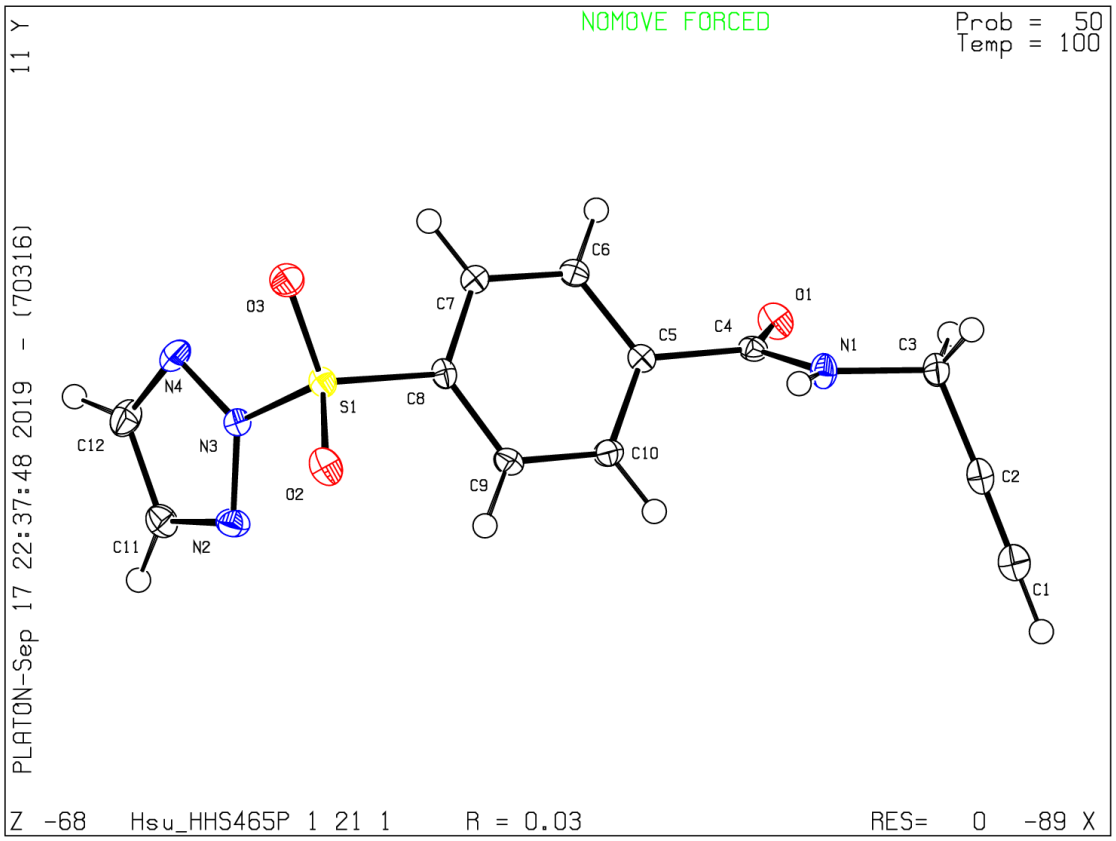
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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

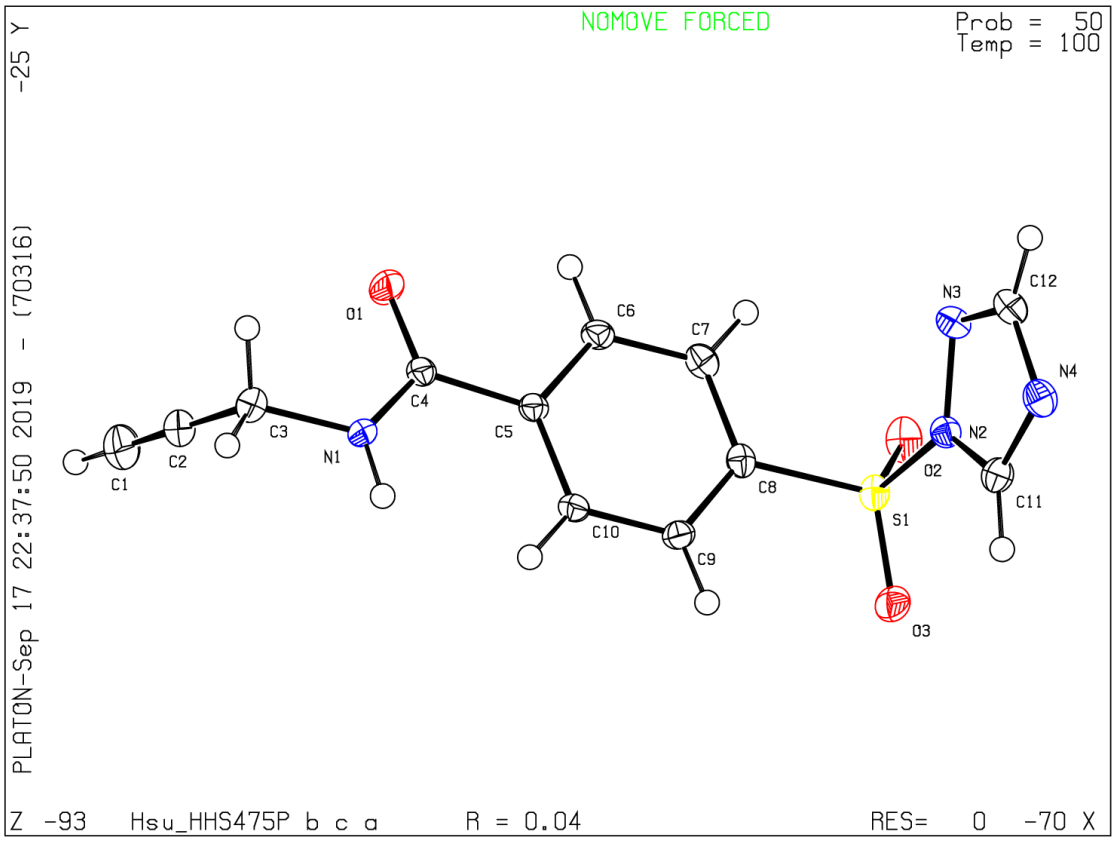
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock Hsu_HHS465 - ellipsoid plot



Datablock Hsu_HHS475 - ellipsoid plot



Datablock Hsu_HHS483 - ellipsoid plot