

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1

Bond precision:	C-C = 0.0104 A	Wavelength=0.71073	
Cell:	a=9.7575(4)	b=12.1470(4)	c=25.8906(10)
	alpha=90	beta=93.963(3)	gamma=90
Temperature:	571 K		
	Calculated	Reported	
Volume	3061.3(2)	3061.3(2)	
Space group	P 21/c	P21/c	
Hall group	-P 2ybc	?	
Moiety formula	C60 H44 Ag2 N8 S4, 2(C F3 O3 S)	C62 H44 Ag2 F6 N8 O6 S6	
Sum formula	C62 H44 Ag2 F6 N8 O6 S6	C62 H44 Ag2 F6 N8 O6 S6	
Mr	1519.15	1519.15	
Dx,g cm-3	1.648	1.648	
Z	2	2	
Mu (mm-1)	0.922	0.922	
F000	1528.0	1528.0	
F000'	1526.55		
h,k,lmax	12,15,33	12,15,33	
Nref	6689	6611	
Tmin,Tmax	0.991,0.991	0.991,0.991	
Tmin'	0.991		

Correction method= # Reported T Limits: Tmin=0.991 Tmax=0.991
AbsCorr = EMPIRICAL

Data completeness= 0.988 Theta(max)= 27.000

R(reflections)= 0.0766(5450) wR2(reflections)= 0.1951(6611)

S = 1.151 Npar= 406

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 B

PLAT241_ALERT_2_B High Ueq as Compared to Neighbors for S2 Check

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for C2 -- C3 .. 5.4 su
PLAT234_ALERT_4_C Large Hirshfeld Difference C3 -- C4 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29 -- C30 .. 0.20 Ang.
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for S1 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C28 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C23 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C27 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C30 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S3 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.0104 Ang.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 7.92 Why ?
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C31 Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
5 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

