

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) md7

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: md7

Bond precision:	C-C = 0.0095 A	Wavelength=0.71073
Cell:	a=13.6834(11) b=8.0480(5) c=15.5345(13)	
	alpha=90 beta=103.199(6) gamma=90	
Temperature:	250 K	
	Calculated	Reported
Volume	1665.5(2)	1665.5(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C15 H11 Ag F3 N3 O3 S	C15 H11 Ag F3 N3 O3 S
Sum formula	C15 H11 Ag F3 N3 O3 S	C15 H11 Ag F3 N3 O3 S
Mr	478.20	478.20
Dx,g cm-3	1.907	1.907
Z	4	4
Mu (mm-1)	1.389	1.389
F000	944.0	944.0
F000'	941.39	
h,k,lmax	16,9,18	16,9,18
Nref	2978	2962
Tmin,Tmax	0.736,0.858	0.562,0.789
Tmin'	0.680	

Correction method= # Reported T Limits: Tmin=0.562 Tmax=0.789
AbsCorr = INTEGRATION

Data completeness= 0.995 Theta(max)= 25.139

R(reflections)= 0.0597(2537) wR2(reflections)= 0.1660(2962)

S = 1.066 Npar= 237

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

PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Ag1	--01	.	9.1 s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			01 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			N3 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			C14 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds			0.00946 Ang.



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	5	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.08	Why ?
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C13	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	34	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	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
 5 **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
- 0 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
 2 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.

PLATON version of 18/02/2019; check.def file version of 18/02/2019

Datablock md7 - ellipsoid plot

