

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AgDIsoFMDThio

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: AgDIsoFMDThio

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Bond precision:    C-C = 0.0068 A                      Wavelength=0.71073

Cell:                      a=30.0941(6)              b=30.0941(6)              c=50.6555(11)  
                                alpha=90                      beta=90                      gamma=120  
Temperature:              100 K

	Calculated	Reported
Volume	39730(2)	39730(2)
Space group	R -3	R -3 :h
Hall group	-R 3	-R 3
Moiety formula	C156 H210 Ag6 N12 S12 [+ solvent]	C156 H210 Ag6 N12 S12
Sum formula	C156 H210 Ag6 N12 S12 [+ solvent]	C156 H210 Ag6 N12 S12
Mr	3285.31	3285.29
Dx, g cm-3	1.236	1.236
Z	9	9
Mu (mm-1)	0.841	0.841
F000	15336.0	15336.0
F000'	15304.62	
h,k,lmax	37,37,63	37,37,62
Nref	18109	17643
Tmin,Tmax	0.809,0.889	0.766,0.902
Tmin'	0.764	

Correction method= # Reported T Limits: Tmin=0.766 Tmax=0.902  
AbsCorr = MULTI-SCAN

Data completeness= 0.974                      Theta(max)= 26.389

R(reflections)= 0.0409( 10880)              wR2(reflections)= 0.1009( 17643)

S = 0.935                      Npar= 862

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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 C

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.6	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range	4.5	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C74	Check	
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-7.154	Report	
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-0.054	Report	
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	255	Report	
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info	



#### Alert level G

PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	205	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	23	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  
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

