

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

Bond precision: C-C = 0.0057 Å Wavelength=0.71073

Cell: a=7.8326(2) b=11.0556(2) c=12.8446(3)
 alpha=114.754(1) beta=102.718(1) gamma=94.914(1)
Temperature: 100 K

	Calculated	Reported
Volume	965.22(4)	965.22(4)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C15 H3 Ag3 F18 N6, C22 H15 N O	C15 H3 Ag3 F18 N6, C22 H15 N O
Sum formula	C37 H18 Ag3 F18 N7 O	C37 H18 Ag3 F18 N7 O
Mr	1242.19	1242.19
Dx, g cm ⁻³	2.137	2.137
Z	1	1
Mu (mm ⁻¹)	1.638	1.638
F000	600.0	600.0
F000'	597.72	
h, k, lmax	9, 13, 15	9, 13, 15
Nref	7580 [3790]	5359
Tmin, Tmax	0.723, 0.877	0.317, 0.380
Tmin'	0.668	

Correction method= # Reported T Limits: Tmin=0.317 Tmax=0.380
AbsCorr = MULTI-SCAN

Data completeness= 1.41/0.71 Theta(max)= 25.998

R(reflections)= 0.0153(5326)	wR2(reflections)= 0.0368(5359)
S = 1.037	Npar= 595

test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

PLAT915_ALERT_3_B No Flack x Check Done: Low Friedel Pair Coverage 42 %

Author Response: The reason is P1 space group. It is impossible to measure all necessary equivalent reflections.

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	6.34	Note
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C9	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact H18 ..H21	1.98	Ang.
	x,y,z =	1_555	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	14 Report

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001 Degree
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3 ..F9 .	2.84 Ang.
	1+x,1+y,z =	1_665 Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	14 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.5 Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 Info

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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
4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
7 ALERT level G = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
0 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.

