

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 190926a_0m_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: 190926a_0m_a

Bond precision:	C-C = 0.0039 A	Wavelength=0.71076
Cell:	a=11.866(12)	b=9.750(11) c=22.08(2)
	alpha=90	beta=102.027(13) gamma=90
Temperature:	296 K	
	Calculated	Reported
Volume	2498(4)	2498(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C56 H50 Ag2 N10 O4, 2(H2 O)	C56 H50 Ag2 N10 O4, 2(H2 O)
Sum formula	C56 H54 Ag2 N10 O6	C56 H54 Ag2 N10 O6
Mr	1178.83	1178.83
Dx, g cm-3	1.567	1.567
Z	2	2
Mu (mm-1)	0.848	0.848
F000	1204.0	1204.0
F000'	1200.83	
h, k, lmax	14, 11, 26	14, 11, 26
Nref	4428	4373
Tmin, Tmax	0.713, 0.737	0.713, 0.737
Tmin'	0.699	

Correction method= # Reported T Limits: Tmin=0.713 Tmax=0.737
AbsCorr = MULTI-SCAN

Data completeness= 0.988 Theta(max)= 25.028

R(reflections)= 0.0278(3596) wR2(reflections)= 0.0665(4373)

S = 1.023 Npar= 334

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

RADNW01_ALERT_1_C The radiation wavelength lies outside the expected range
for the supplied radiation type. Expected range 0.71065-0.71075
Wavelength given = 0.71076

PLAT148_ALERT_3_C s.u. on the	a	- Axis is (Too) Large	0.012 Ang.
PLAT148_ALERT_3_C s.u. on the	b	- Axis is (Too) Large	0.0110 Ang.
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent			1 Check
00AA			
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag01	--N1		8.4 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of			01 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).			5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=	0.595		49 Report



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	2 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	4 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	63% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	50 Note
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
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **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
- 3 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
6 ALERT type 3 Indicator that the structure quality may be low
1 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.

