

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 = 0.0090 A	Wavelength=0.71073
Cell:	a=13.1222 (8)	b=14.3897 (10) c=20.6671 (14)
	alpha=90	beta=91.486 (3) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	3901.1 (4)	3901.1 (4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C37 H18 Ag3 F18 N7 O	C37 H18 Ag3 F18 N7 O
Sum formula	C37 H18 Ag3 F18 N7 O	C37 H18 Ag3 F18 N7 O
Mr	1242.20	1242.19
Dx, g cm ⁻³	2.115	2.115
Z	4	4
Mu (mm ⁻¹)	1.621	1.621
F000	2400.0	2400.0
F000'	2390.87	
h, k, lmax	16, 17, 25	16, 17, 25
Nref	7656	7611
Tmin, Tmax	0.747, 0.837	0.245, 0.380
Tmin'	0.711	

Correction method= # Reported T Limits: Tmin=0.245 Tmax=0.380
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.998

R(reflections)= 0.0424 (7068)	wR2(reflections)= 0.0978 (7611)
S = 1.151	Npar= 604

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

PLAT213_ALERT_2_C	Atom F00J	has ADP max/min Ratio	3.7	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 Ag Ueq(max)/Ueq(min) Range	3.6	Ratio
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.00903	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		3.226	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	44	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H01L	.	-0.47	eA-3



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		1	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		30.53	Why ?
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag4 --N1	.	12.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag4 --N6	.	12.7	s.u.
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C016	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C017	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C01G	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C01H	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C01S	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ag1	Constrained at	0.95	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ag4	Constrained at	0.05	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	2%	Note
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F008 ..F00J	.	2.79	Ang.
	-l+x,y,z =		1_455	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		75	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		6	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		12	Note
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.		0	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
21 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 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
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* 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.

