

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 000

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: 000

Bond precision:	C-C = 0.0036 A	Wavelength=0.71073	
Cell:	a=27.0362 (12) alpha=90	b=27.0362 (12) beta=90	c=18.5958 (18) gamma=120
Temperature:	153 K		
	Calculated	Reported	
Volume	11771.6 (15)	11771.6 (15)	
Space group	R -3	R -3	
Hall group	-R 3	-R 3	
Moiety formula	2 (C81 H72 Ag3 N15 O6), 7.5 (C2 H6 O)	2 (C81 H72 Ag3 N15 O6), 7.5 (C2 H6 O)	
Sum formula	C177 H189 Ag6 N30 O19.50	C177 H189 Ag6 N30 O19.50	
Mr	3695.81	3695.79	
Dx, g cm-3	1.564	1.564	
Z	3	3	
Mu (mm-1)	0.814	0.814	
F000	5697.0	5697.0	
F000'	5682.82		
h, k, lmax	32, 32, 22	32, 32, 22	
Nref	4607	4589	
Tmin, Tmax	0.718, 0.740	0.718, 0.740	
Tmin'	0.703		

Correction method= # Reported T Limits: Tmin=0.718 Tmax=0.740
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.021

R(reflections)= 0.0266 (4065)

wR2(reflections)=
0.0696 (4589)

S = 1.042

Npar= 362

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) Agl --O1 . 5.8 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 01 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 04 0.140 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 17 Report
0 3 0, -2 4 0, -3 6 0, -2 3 1, 1 3 1, -4 4 1,
-1 4 1, 1 2 2, -3 4 2, 0 4 2, 0 0 3, -3 3 3,
-1 5 3, -2 2 5, 1 2 5, -1 3 5, 0 0 6,



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 3 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
H3A H4A
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 34.58 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O4 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C30 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31 Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31B Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31C Constrained at 0.25 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 3) 2.25 Check
PLAT411_ALERT_2_G Short Inter H...H Contact H23 ..H30A . 1.76 Ang.
-1/3+y,1/3-x+y,1/3-z = 14_455 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H23 ..H31B . 1.87 Ang.
-x+y,1-x,z = 3_565 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H24 ..H31B . 2.11 Ang.
-x+y,1-x,z = 3_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C26 ..C30 . 3.12 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C27 ..C31 . 3.19 Ang.
-x+y,1-x,z = 3_565 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 9 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers 1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 33 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 78% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
-1 1 1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 18 Note
-4 4 1, -3 3 3, -3 4 2, -3 6 0, -2 2 5, -2 3 1,

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-2  4  0, -1  1  1, -1  3  5, -1  4  1, -1  5  3,  0  0  3,
  0  0  6,  0  3  0,  0  4  2,  1  2  2,  1  2  5,  1  3  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.771 Note
      Predicted wR2: Based on SigI**2  2.51 or SHELX Weight  6.68
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 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
4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
35 ALERT level G = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 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
17 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

