

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20wd_wvz_wd4_agbpymtci_0m1

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: 20wd_wvz_wd4_agbpymtci_0m1

Bond precision: C-C = 0.0065 Å Wavelength=0.71073

Cell: a=28.2245 (7) b=7.1755 (2) c=27.6678 (7)
 alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	5603.4 (3)	5603.4 (3)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C48 H46 Ag4 N8 O4 S2, 2 (F6 P)	C48 H46 Ag4 N8 O4 S2, 2 (F6 P)
Sum formula	C48 H46 Ag4 F12 N8 O4 P2 S2	C48 H46 Ag4 F12 N8 O4 P2 S2
Mr	1584.47	1584.47
Dx, g cm ⁻³	1.878	1.878
Z	4	4
Mu (mm ⁻¹)	1.600	1.600
F000	3120.0	3120.0
F000'	3108.95	
h, k, lmax	37, 9, 36	37, 9, 36
Nref	13822 [7054]	13261
Tmin, Tmax		0.575, 0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.575 Tmax=0.746
AbsCorr = NONE

Data completeness= 1.88/0.96 Theta(max)= 28.203

R(reflections)= 0.0245 (12163)

wR2(reflections)=
0.0518 (13261)

S = 1.052

Npar= 725

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 B

PLAT109_ALERT_2_B Twinning Matrix is inverted Laue group operation ? Check



Alert level C

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C01U Check
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by -0.0017 Check
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by -0.0042 Check



Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag01 --S005 . 20.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag01 --S006 . 9.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag02 --S005 . 10.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag02 --S006_b . 21.2 s.u.
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P007 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P008 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 126 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 34 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.50 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

14 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

9 ALERT type 2 Indicator that the structure model may be wrong or deficient

1 ALERT type 3 Indicator that the structure quality may be low

4 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

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.

