

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20200929jiangshicun2_0m

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: 20200929jiangshicun2_0m

Bond precision: C-C = 0.0026 Å Wavelength=1.54178

Cell: a=5.8374(1) b=15.9288(4) c=21.4209(5)
 alpha=90 beta=93.903(1) gamma=90
Temperature: 273 K

	Calculated	Reported
Volume	1987.16(8)	1987.16(8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H16 F 02 P [+ solvent]	C21 H16 F 02 P
Sum formula	C21 H16 F 02 P [+ solvent]	C21 H16 F 02 P
Mr	350.31	350.31
Dx, g cm ⁻³	1.171	1.171
Z	4	4
Mu (mm ⁻¹)	1.386	1.386
F000	728.0	728.0
F000'	731.31	
h, k, lmax	7, 19, 26	7, 19, 26
Nref	3910	3889
Tmin, Tmax		0.311, 0.754
Tmin'		

Correction method= # Reported T Limits: Tmin=0.311 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 72.101

R(reflections)= 0.0477(3734) wR2(reflections)= 0.1346(3889)

S = 1.030 Npar= 226

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

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
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	17 Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	9 Note

● Alert level G

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	273 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	273 Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O2	105.5 Degree
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	184 A**3
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	4 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
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT053_20200929jiangshicun2_0m
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT054_20200929jiangshicun2_0m
;
PROBLEM: Medium Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT055_20200929jiangshicun2_0m
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT911_20200929jiangshicun2_0m
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600          17 Report
RESPONSE: ...
;
_vrf_PLAT913_20200929jiangshicun2_0m
;
PROBLEM: Missing # of Very Strong Reflections in FCF ....      9 Note
RESPONSE: ...
;
# end Validation Reply Form
```

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.

