

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: Jiang20230309

Bond precision:	C-C = 0.0035 A	Wavelength=1.54184
Cell:	a=41.2828 (12) alpha=90	b=6.2666 (2) beta=99.943 (3)
Temperature:	93 K	c=41.4397 (12) gamma=90
	Calculated	Reported
Volume	10559.5 (6)	10559.5 (6)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C20 H22 B F O2	?
Sum formula	C20 H22 B F O2	C20 H22 B F O2
Mr	324.19	324.18
Dx, g cm ⁻³	1.224	1.224
Z	24	24
Mu (mm ⁻¹)	0.673	0.673
F000	4128.0	4128.0
F000'	4140.53	
h, k, lmax	50, 7, 51	50, 7, 50
Nref	10638	10362
Tmin, Tmax	0.960, 0.993	0.885, 1.000
Tmin'	0.935	

Correction method= # Reported T Limits: Tmin=0.885 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.974 Theta(max)= 73.522

R(reflections)= 0.0569 (6824)	wR2(reflections)=
S = 1.048	0.1892 (10362)
Npar= 661	

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for F3 --C42 . 12.3 s.u.

Author Response: Resolving disorders on F3 has been attempted, but none of disorders around F3 could be located. The chemical structure of this compound as C-F species has been confirmed by other spectroscopic methods.



Alert level G

PLAT012_ALERT_1_G	N.O.K.	_shelx_res_checksum	Found in CIF		Please Check
PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle From 120 for O1	.	106.8 Degree
PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle From 120 for O2	.	106.4 Degree
PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle From 120 for O3	.	107.0 Degree
PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle From 120 for O4	.	107.3 Degree
PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle From 120 for O5	.	107.2 Degree
PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle From 120 for O6	.	107.2 Degree
PLAT941_ALERT_3_G	Average HKL Measurement	Multiplicity		3.6	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT	Optimisation	has not Converged		Please Check

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
0 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

