

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: grot304

Bond precision:	C-C = 0.0056 A	Wavelength=0.71073
Cell:	a=11.9277(7) b=19.2100(11) c=28.2172(16)	
	alpha=90 beta=90 gamma=90	
Temperature:	120 K	
	Calculated	Reported
Volume	6465.4(6)	6465.4(6)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	2(C23 H32 Cl Ir N3), 2(F6 P), 3(C4 H8 O)	C23 H32 Cl Ir N3, F6 P, 1.5(C4 H8 O)
Sum formula	C58 H88 Cl2 F12 Ir2 N6 O3 P2	C29 H44 Cl F6 Ir N3 O1.50 P
Mr	1662.62	831.29
Dx, g cm ⁻³	1.708	1.708
Z	4	8
Mu (mm ⁻¹)	4.326	4.326
F000	3312.0	3312.0
F000'	3304.23	
h,k,lmax	16,25,37	15,25,36
Nref	8234	7090
Tmin,Tmax	0.440,0.621	0.411,0.648
Tmin'	0.336	

Correction method= # Reported T Limits: Tmin=0.411 Tmax=0.648
AbsCorr = MULTI-SCAN

Data completeness= 0.861 Theta(max)= 28.551

R(reflections)= 0.0287(5367) wR2(reflections)= 0.0563(7090)

S = 1.022 Npar= 417

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 A**

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.899 Why?

Author Response: Failure in low-T device corrupted the last data collection run

 **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	11.85	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		P1 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	57%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1S	105.0	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O2S	107.7	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact F2B ..C5S	2.90	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	12	Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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.

PLATON version of 13/12/2017; check.def file version of 12/12/2017

