

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ver0-9205_mk-264

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: ver0-9205_mk-264

Bond precision: C-C = 0.0061 A

Wavelength=0.71070

Cell: a=9.8380(3) b=11.1732(4) c=11.5835(6)
 alpha=69.378(4) beta=69.344(4) gamma=89.336(3)
Temperature: 100 K

	Calculated	Reported
Volume	1105.82(9)	1105.82(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C15 H14 N4 O, C6 F4 I2	C6 F4 I2, C15 H14 N4 O
Sum formula	C21 H14 F4 I2 N4 O	C21 H14 F4 I2 N4 O
Mr	668.16	668.16
Dx,g cm-3	2.007	2.007
Z	2	2
Mu (mm-1)	2.899	2.899
F000	636.0	636.0
F000'	634.41	
h,k,lmax	13,14,15	13,14,15
Nref	5611	5603
Tmin,Tmax	0.599,0.748	0.724,1.000
Tmin'	0.588	

Correction method= # Reported T Limits: Tmin=0.724 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 28.499

R(reflections)= 0.0363(4709)

wR2(reflections)= 0.0817(5603)

S = 1.054

Npar= 290

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**

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.03	Report
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.833	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	5	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.83A From I2S	2.16	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.87A From I1S	1.70	eA-3

● **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
PLAT431_ALERT_2_G	Short Inter HL..A Contact I1S ..N1 .	2.99	Ang.
	1-x,2-y,1-z =	2_676	Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact I2S ..N4 .	2.97	Ang.
	x,y,z =	1_555	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.	6	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **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
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

