

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 11

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: 11

Bond precision: C-C = 0.0127 Å Wavelength=1.54178

Cell: a=8.5944(2) b=9.9487(2) c=14.6476(4)
 alpha=75.949(1) beta=83.172(1) gamma=89.966(1)

Temperature: 173 K

	Calculated	Reported
Volume	1205.81(5)	1205.81(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C11 H10 I N3 O2	C11 H10 I N3 O2
Sum formula	C11 H10 I N3 O2	C11 H10 I N3 O2
Mr	343.12	343.12
Dx,g cm-3	1.890	1.890
Z	4	4
Mu (mm-1)	20.840	20.840
F000	664.0	664.0
F000'	664.76	
h,k,lmax	10,12,18	10,12,17
Nref	4755	4628
Tmin,Tmax	0.075,0.067	0.112,0.366
Tmin'	0.012	

Correction method= # Reported T Limits: Tmin=0.112 Tmax=0.366
AbsCorr = NUMERICAL

Data completeness= 0.973 Theta(max)= 72.104

R(reflections)= 0.0621(4290) wR2(reflections)= 0.1709(4628)

S = 1.067 Npar= 310

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**

PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01272	Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N6 --H6B .		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.562	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	77	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.45A From I1	2.28	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.18A From C8	2.10	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.47A From I2	2.06	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 2.05A From I1	1.96	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.76A From C11	1.93	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.09A From C7	1.90	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.41A From C10	1.83	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.99A From I2	1.81	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.86A From I1	-1.57	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H6B	-0.31	eA-3

● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	16.83	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	47	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.5	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
14 **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

1 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
13 **ALERT type 2** Indicator that the structure model may be wrong or deficient
5 **ALERT type 3** Indicator that the structure quality may be low
1 **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 03/06/2021; check.def file version of 02/06/2021

