



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rudi005

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: rudi005

Bond precision:	C-C = 0.0113 Å	Wavelength=1.54178	
Cell:	a=11.2013 (3)	b=16.6942 (4)	c=22.1759 (6)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	4146.82 (19)	4146.82 (19)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C36 H52 N, I4 In	C36 H52 N, I4 In	
Sum formula	C36 H52 I4 In N	C36 H52 I4 In N	
Mr	1121.21	1121.20	
Dx, g cm ⁻³	1.796	1.796	
Z	4	4	
Mu (mm ⁻¹)	28.093	28.093	
F000	2144.0	2144.0	
F000'	2145.69		
h, k, lmax	14, 20, 27	13, 20, 27	
Nref	8474 [4714]	8254	
Tmin, Tmax	0.063, 0.161	0.326, 0.754	
Tmin'	0.010		

Correction method= # Reported T Limits: Tmin=0.326 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 1.75/0.97 Theta(max)= 74.555

R(reflections)= 0.0374(8086)

wR2(reflections)=
0.1002(8254)

S = 1.040

Npar= 392

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 0.01131 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 20 Report
8 0 0, 13 1 0, 13 2 0, 13 3 0, 13 4 0, 13 5 0,
13 0 1, 13 1 1, 13 2 1, 13 3 1, 13 4 1, 13 5 1,
13 0 2, 0 1 2, 13 1 2, 13 4 2, 13 1 3, 6 0 14,
0 0 26, 0 4 26,
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.75Ang From In1 -2.00 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.69Ang From I3 -1.94 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.75Ang From I1 -1.85 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.69Ang From I1 -1.78 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.74Ang From I3 -1.73 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From I4 -1.72 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From I2 -1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From In1 -1.57 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.01Ang From I1 -1.57 eA-3

● **Alert level G**

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 37 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 10.47 Why ?
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0020 Report
PLAT794_ALERT_5_G Tentative Bond Valency for In1 (III) . 3.25 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 525 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 26 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 11 Note
-4 -1 -1, -2 -3-27, -1 -8-25, 0 1 2, 0 4 26, 1 1 1,
6 0 14, 8 0 0, 8 8 19, 13 1 3, 13 3 1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.254 Note
Predicted wR2: Based on SigI**2 4.45 or SHELX Weight 9.64 Note
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
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected
- 0 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
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

Datablock rudi005 - ellipsoid plot

