



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rudi006

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: rudi006

Bond precision: C-C = 0.0045 Å

Wavelength=1.54178

Cell: a=15.4516(5) b=15.9289(5) c=16.4252(6)
 alpha=105.997(1) beta=114.897(1) gamma=105.715(1)
Temperature: 100 K

	Calculated	Reported
Volume	3159.02(19)	3159.02(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C H B11 Cl11, C9 H23 In N3	1(C9 H23 In N3), C H B11 Cl11
Sum formula	C10 H24 B11 Cl11 In N3	C10 H24 B11 Cl11 In N3
Mr	810.00	810.00
Dx, g cm ⁻³	1.703	1.703
Z	4	4
Mu (mm ⁻¹)	14.629	14.629
F000	1584.0	1584.0
F000'	1602.51	
h, k, lmax	19, 19, 20	19, 19, 20
Nref	12945	12696
Tmin, Tmax	0.073, 0.145	0.322, 0.754
Tmin'	0.017	

Correction method= # Reported T Limits: Tmin=0.322 Tmax=0.754
AbsCorr = MULTISCAN

Data completeness= 0.981

Theta(max)= 74.473

R(reflections)= 0.0365(12030)

wR2(reflections)=
0.0974(12696)

S = 1.047

Npar= 752

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
Calc: C H B11 Cl11, C9 H23 In N3		
Rep.: 1(C9 H23 In N3), C H B11 Cl11		
PLAT601_ALERT_2_C	Unit-Cell Contains Solvent Accessible VOIDS .LE.	35 Ang**3
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	41 Report
2 0 0, 0 2 0, -1 -3 1, 0 -2 2, 13-16 3, -1 -5 3,		
-16 -1 3, 12-16 4, 13-15 4, 14-13 4, -5 -1 4, -12 16 4,		
11-16 5, 12-16 5, 12-15 5, 13-13 5, 0 -4 5, -4 0 5,		
-12 16 5, -13 -8 6, -14 -6 6, -15 -4 6, -12 15 6, -13 -8 7,		
-14 -7 7, -15 -5 7, -12 15 7, -12-10 8, -12 14 8, 10-10 10,		
(11 More NOT listed: see .ckf listing file)		
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.78Ang From In1	-2.00 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.78Ang From In2	-1.99 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.87Ang From In2	-1.88 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.79Ang From In1	-1.62 eA-3



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	25 Note					
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	21 Report					
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.06 Why ?					
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001 Degree					
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C2A	3.14 Check					
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2 Note					
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	6 Report					
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					
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0020 Report					
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0020 Report					
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0020 Report					
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0020 Report					
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0020 Report					
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0020 Report					
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	69% Note					
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C19 Check					
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C20 Check					
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	23 Note					
H1AA	H1AB	H2AA	H2AB	H3AA	H3AB	H4AA	H4AB
H5AA	H5AB	H5AC	H6AA	H6AB	H6AC	H7AA	H7AB
H7AC	H8AA	H8AB	H8AC	H9AA	H9AB	H9AC	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	477 Note					

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 207 Note
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 10 Note
 -15 16 1, -5 -1 4, -4 0 5, -1 -5 3, -1 -3 1, 0 -4 5,
 0 -2 2, 0 2 0, 2 0 0, 4 -4 0,
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.463 Note
 Predicted wR2: Based on SigI**2 2.81 or SHELX Weight 9.31 Note
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 8 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. 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

