



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rudi003

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: rudi003

Bond precision: C-C = 0.0050 Å

Wavelength=1.54178

Cell: a=12.1607 (5) b=12.7895 (5) c=17.5910 (8)
 alpha=94.759 (2) beta=92.161 (2) gamma=112.200 (2)
Temperature: 100 K

	Calculated	Reported
Volume	2517.29 (19)	2517.29 (19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C35 H49 In N, C H B11 Cl11	C35 H49 In N, C H B11 Cl11
Sum formula	C36 H50 B11 Cl11 In N	C36 H50 B11 Cl11 In N
Mr	1120.45	1120.45
Dx, g cm ⁻³	1.478	1.478
Z	2	2
Mu (mm ⁻¹)	9.339	9.339
F000	1128.0	1128.0
F000'	1137.94	
h, k, lmax	15, 15, 21	15, 15, 21
Nref	10313	10127
Tmin, Tmax	0.178, 0.281	0.470, 0.754
Tmin'	0.079	

Correction method= # Reported T Limits: Tmin=0.470 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.982

Theta(max)= 74.677

R(reflections)= 0.0413(9270)

wR2(reflections)=
0.1100(10127)

S = 1.037

Npar= 553

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	4.7	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	4.8	Ratio
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours			C30	Check
PLAT351_ALERT_3_C	Long	C-H (X0.96,N1.08A)	C36	- H36	.	1.12	Ang.
PLAT911_ALERT_3_C	Missing FCF	Refl Between Thmin & STh/L=	0.600			41	Report
	-1 1 1,	-1 14 1,	-4 0 3,	-14 4 3,	0-14 4,	1-14 4,	
	-14 2 4,	-14 3 4,	-14 4 4,	-2 14 4,	0-14 5,	1-14 5,	
	2-14 5,	-14 4 5,	-2 14 5,	1-14 6,	2-14 6,	-1 13 6,	
	1-14 7,	-1-13 7,	0-13 7,	-1 13 7,	-3-12 8,	0 12 8,	
	-4-11 9,	-1 12 9,	-12 0 10,	-1 12 10,	2-11 15,	3-11 15,	
	(11 More NOT listed: see .ckf listing file)						
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.72Ang	From Inl			-1.57	eA-3



Alert level G

PLAT083_ALERT_2_G	SHELXL	Second Parameter in WGHT	Unusually Large	7.05	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles	are Equal ..(Note)	0.002	Degree	
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Inl --N1	5.7	s.u.	
PLAT308_ALERT_2_G	Single Bonded Metal Atom	in Structure (Unusual)	Inl	Check	
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C36	Check	
PLAT912_ALERT_4_G	Missing # of FCF Reflections	Above STh/L= 0.600	144	Note	
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections	in FCF	2	Note	
	-1 1 1,	-4 0 3,			
PLAT933_ALERT_2_G	Number of HKL-OMIT Records	in Embedded .res File	3	Note	
	-4 0 3,	-1 1 1,	12 3 5,		
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		3.815	Note	
	Predicted wR2: Based on SigI**2 2.88 or SHELX Weight 10.61				
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		7	Info	
PLAT994_ALERT_1_G	SHELXL .ins Contains no or MERG 0 Instruction	..	!	Note	

- 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
11 **ALERT level G** = General information/check it is not something unexpected

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

Datablock rudi003 - ellipsoid plot

