checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rudi001

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: rudi001

```
Bond precision:   B- B = 0.0050 A          Wavelength=1.54178

Cell:              a=10.3212(3)      b=13.0627(3)      c=20.4914(5)
                   alpha=90          beta=90           gamma=90
Temperature:       100 K
```

	Calculated	Reported
Volume	2762.71(12)	2762.71(12)
Space group	P n m a	Pnma
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	2(C H B11 Cl11), 4(C3 H4.50 N1.50 Ni0.25)	C12 H18 N6 Ni, 2(C H B11 Cl11)
Sum formula	C14 H20 B22 Cl22 N6 Ni	C14 H20 B22 Cl22 N6 Ni
Mr	1348.77	1348.79
Dx,g cm-3	1.621	1.621
Z	2	2
Mu (mm-1)	10.516	10.516
F000	1316.0	1316.0
F000'	1327.53	
h,k,lmax	12,16,25	12,16,25
Nref	2959	2943
Tmin,Tmax	0.191,0.250	0.406,0.754
Tmin'	0.053	

```
Correction method= # Reported T Limits: Tmin=0.406 Tmax=0.754
AbsCorr = MULTI-SCAN
```

Data completeness= 0.995 Theta(max)= 74.583

R(reflections)= 0.0417(2843) wR2(reflections)= 0.1157(2943)

S = 1.201 Npar= 236

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 B

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density .... 5.13 Report

Author Response: An artefactual peak that does not make chemical sense is located near the nickel atom perhaps resulting from less-than-ideal absorption correction.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: 2(C H B11 Cl11), 4(C3 H4.50 N1.50 Ni0.25)
Rep.: C12 H18 N6 Ni, 2(C H B11 Cl11)

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 2.29 eA-3

PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C9 - H9 . 1.12 Ang.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.973 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 10 Report
2 0 0, 4 0 0, 2 1 0, 0 2 0, 2 1 1, 2 1 2,
0 2 2, 0 0 4, 0 4 4, 2 0 5,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.25Ang From Ni1 2.17 eA-3

PLAT977_ALERT_2_C Check Negative Difference Density on H9 . -0.31 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 13 Note

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 13 Report

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.89 Why ?

PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR 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 0.0010 Report

PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0010 Report

PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0010 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

PLAT299_ALERT_4_G Atom Site Occupancy Constrained at ..... 0.5 Check
N2 N4 C3 C4 C7 C8 H4A H4B

```
             H4C     H8A     H8B     H8C
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............       0.25 Check
             Ni1     N1      N3      C1      C2      C5      C6      H2A
             H2B     H2C     H6A     H6B     H6C
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       9.25 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C9 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1      ..Cl7      .       3.38 Ang.
                                                  -1+x,y,z  =      1_455 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl5      ..Cl5      .       3.39 Ang.
                                               1-x,1-y,1-z  =      5_666 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         25 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         13 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       148 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=       4.80 Note
               0  1  1,   0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
               4  0  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         12 Note
               0  0  2,   0  0  4,   0  1  1,   0  2  0,   0  2  2,   0  4  4,
               2  0  0,   2  0  5,   2  1  0,   2  1  1,   2  1  2,   4  0  0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.059 Note
             Predicted wR2: Based on SigI**2  2.29 or SHELX Weight  9.64
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
  1 ALERT level B = A potentially serious problem, consider carefully
  8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 30 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 12 ALERT type 3 Indicator that the structure quality may be low
 11 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 15/01/2026; check.def file version of 02/01/2026

---

duplicate check

No duplication found

Datablock rudi001 - ellipsoid plot