

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: NiGd

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Bond precision:    C-C = 0.0061 A

Wavelength=0.71073

Cell:                    a=15.9042(5)            b=12.9690(3)            c=21.7691(6)  
                          alpha=90                beta=111.352(3)        gamma=90  
Temperature:            100 K

	Calculated	Reported
Volume	4181.9(2)	4181.9(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C50 H90 Gd2 Ni2 O22, 2(C6 H16 N), 2(C2 H3 N)	C50 H90 Gd2 Ni2 O22, 2(C6 H16 N), 2(C2 H3 N)
Sum formula	C66 H128 Gd2 N4 Ni2 O22	C66 H128 Gd2 N4 Ni2 O22
Mr	1761.60	1761.64
Dx,g cm-3	1.399	1.399
Z	2	2
Mu (mm-1)	2.074	2.074
F000	1824.0	1824.0
F000'	1825.40	
h,k,lmax	19,16,27	19,16,27
Nref	8561	8550
Tmin,Tmax	0.819,0.901	0.580,1.000
Tmin'	0.813	

Correction method= # Reported T Limits: Tmin=0.580 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 26.372

R(reflections)= 0.0321( 7655)

wR2(reflections)= 0.0795( 8550)

S = 1.031

Npar= 453

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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	Large Non-Solvent	C	Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT242_ALERT_2_C	Low		Ueq as Compared to Neighbors for .....	C2	Check



### Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	10	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	11.87	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2 -- C3 ..	5.7	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2 -- C4 ..	9.0	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2 -- C5 ..	10.0	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2 -- C10 ..	8.7	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2 -- C1P ..	6.3	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2 -- C1R ..	9.3	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C12 -- C13 ..	9.7	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C12 -- C14 ..	8.0	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C12 -- C1Q ..	6.0	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C12 -- C1S ..	10.0	su
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) C26 -- C27 ..	6.3	su
PLAT300_ALERT_4_G	Atom Site Occupancy of >C3 is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C4 is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C5 is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C13 is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C14 is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C15 is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1A is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C10 is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1P is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1Q is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1R is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1S is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C3_a is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C4_a is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C5_a is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C13_a is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C14_a is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C15_a is Constrained at	0.794	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1A_a is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C10_a is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1P_a is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1Q_a is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1R_a is Constrained at	0.206	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1S_a is Constrained at	0.206	Check
PLAT301_ALERT_3_G	Main Residue Disorder ..... Percentage =	16	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	18	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.14	Ratio
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	54	Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
14 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
28 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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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*, 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.

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**PLATON version of 29/01/2015; check.def file version of 29/01/2015**

