

## 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: 20191011-CZL-PY-2-2

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Bond precision:	C-C = 0.0187 Å	Wavelength=0.71073	
Cell:	a=20.5601(7) alpha=90	b=20.5601(7) beta=90	c=32.526(3) gamma=120
Temperature:	153 K		
	Calculated	Reported	
Volume	11907.3(14)	11907.2(13)	
Space group	R -3	R -3 :H	
Hall group	-R 3	-R 3	
Moiety formula	C144 H114 Cl13 N12 Ni6 O30 Tb7, 2(C1)	C144 H114 Cl13 N12 Ni6 O30 Tb7, 2(C1)	
Sum formula	C144 H114 Cl15 N12 Ni6 O30 Tb7	C144 H114 Cl15 N12 Ni6 O30 Tb7	
Mr	4488.88	4488.92	
Dx, g cm <sup>-3</sup>	1.878	1.878	
Z	3	3	
Mu (mm <sup>-1</sup> )	4.090	4.090	
F000	6540.0	6540.0	
F000'	6551.35		
h, k, lmax	24, 24, 38	24, 22, 38	
Nref	4684	4671	
Tmin, Tmax	0.374, 0.479	0.374, 0.479	
Tmin'	0.346		

Correction method= # Reported T Limits: Tmin=0.374 Tmax=0.479

AbsCorr = MULTII-SCAN

Data completeness= 0.997

Theta(max)= 25.019

R(reflections)= 0.0595( 3601)

wR2(reflections)=  
0.1639( 4671)

S = 1.038

Npar= 358

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	5.0	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 1	Cl	Ueq(max)/Ueq(min)	Range	5.4	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	6.7	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test	Diff for	O3	--C13	.	5.3	s.u.
PLAT232_ALERT_2_C	Hirshfeld Test	Diff (M-X)	Ni1	--N1	.	5.7	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld	Difference	N1	--C14	.	0.24	Ang.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		C14	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		O3	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		N1	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C22	Check	
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including			Cl4	0.252	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including			Cl4'	0.251	Check
PLAT303_ALERT_2_C	Full Occupancy	Atom H13C	with # Connections			1.13	Check
PLAT342_ALERT_3_C	Low Bond Precision	on C-C Bonds	.....			0.01865	Ang.
PLAT420_ALERT_2_C	D-H Bond Without	Acceptor	Cl3	--H13C	.		Please Check



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note	
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrainted non-H Atoms ...	39	Report	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	3	Report	
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	397.96	Why ?	
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	5	Report	
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	3	Report	
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	5	Report	
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	5	Report	
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report	
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report	
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report	
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report	
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0200	Report	
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0200	Report	
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0200	Report	
PLAT300_ALERT_4_G	Atom Site Occupancy of Tb2	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl3	Constrained at	0.1333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl3'	Constrained at	0.1	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O5	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O5'	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4	Constrained at	0.1667	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4'	Constrained at	0.1667	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	8%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )	0.17 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )	0.17 Check
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H13C ..05' .	2.65 Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H13C ..CL3 .	2.88 Ang.
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	35 Do !
	NI1 -N1 -C14 -C15 -101.00 20.00 1_555 1_555 1_555 1_555	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.11 Ratio
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3 Note
	C1	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	311 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.3 Low
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2 Units
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0 Degree

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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  
 15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 41 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 16 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  
 23 ALERT type 4 Improvement, methodology, query or suggestion  
 3 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* or *IUCrData*, 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.

