

# 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: shelx\_Sam\_AH166

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Bond precision:	C-C = 0.0151 A	Wavelength=0.71073
Cell:	a=10.5126(5)	b=18.8316(10)      c=12.7477(5)
	alpha=90	beta=97.445(5)      gamma=90
Temperature:	120 K	
	Calculated	Reported
Volume	2502.4(2)	2502.4(2)
Space group	P 21/n	P 21/n
Hall group	: -P 2yn	-P 2yn
Moiety formula	C39 H42 Cl3 N9 Nd2 O18	?
Sum formula	C39 H42 Cl3 N9 Nd2 O18	C39 H42 Cl3 N9 Nd2 O18
Mr	1319.65	1319.64
Dx,g cm-3	1.751	1.751
Z	2	2
Mu (mm-1)	2.291	2.291
F000	1308.0	1308.0
F000'	1308.67	
h,k,lmax	12,22,15	12,22,15
Nref	4438	4419
Tmin,Tmax	0.872,0.892	0.772,1.000
Tmin'	0.833	

Correction method= # Reported T Limits: Tmin=0.772 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.996      Theta(max)= 25.040

R(reflections)= 0.0718( 3048)      wR2(reflections)= 0.1808( 4419)

S = 1.061      Npar= 334

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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	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference N1D	--C2D	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N11D	--C12D	0.18	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N1D	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N21D	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C1	Check	
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.01511	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C2	- C3	1.53	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C5	- C6	1.53	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C12	- C16_b	1.53	Ang.



### Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		14	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		2	Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		27.49	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		3	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C11	--C1	9.3	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C1	--C100	9.3	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of C11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C111	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N100	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N111	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N400	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C100	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C111	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C400	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )		10%	Note
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1	-C6	1.45	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C11	-C16	1.46	Ang.
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C2D	Check	
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C3D	Check	
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C12D	Check	
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C13D	Check	
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C22D	Check	
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C23D	Check	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		6	Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C11	--C111	1.71	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Nd1	(II)	2.14	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		48	Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
10 **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

- 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  
3 ALERT type 3 Indicator that the structure quality may be low  
21 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. 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.

