

# 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: 1

---

Bond precision:    C-C = 0.0043 Å                      Wavelength=0.71073

Cell:                      a=15.741(2)              b=10.8220(15)              c=19.530(3)  
                                alpha=90              beta=112.302(2)              gamma=90

Temperature:              273 K

	Calculated	Reported
Volume	3078.1(7)	3078.1(7)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C35 H37 N O4	?
Sum formula	C35 H37 N O4	C35 H38 N O4
Mr	535.66	536.66
Dx,g cm-3	1.156	1.158
Z	4	4
Mu (mm-1)	0.075	0.075
F000	1144.0	1148.0
F000'	1144.51	
h,k,lmax	18,12,23	18,12,23
Nref	5419	5404
Tmin,Tmax	0.981,0.984	
Tmin'	0.981	

Correction method= Not given

Data completeness= 0.997                      Theta(max)= 24.999

R(reflections)= 0.0594( 2868)              wR2(reflections)= 0.1707( 5404)

S = 0.977                      Npar= 368

---

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	1.00	Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.51	Report
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	5.7	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	6.6	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C5 --C6	5.5	s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C4	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C11	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C17	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C33	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C34	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00434	Ang.

## ● Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
Atom count from \_chemical\_formula\_sum: C35 H38 N1 O4  
Atom count from the \_atom\_site data: C35 H37 N1 O4

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G WARNING: H atoms missing from atom site list. Is this intentional?  
From the CIF: \_cell\_formula\_units\_Z 4  
From the CIF: \_chemical\_formula\_sum C35 H38 N O4  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	140.00	140.00	0.00
H	152.00	148.00	4.00
N	4.00	4.00	0.00
O	16.00	16.00	0.00

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .... (K)	273	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .... (K)	273	Check
PLAT793_ALERT_4_G	Model has Chirality at C15 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C29 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C31 (Centro SPGR)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !	
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	9	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.8	Low

---

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

8 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
12 **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  
4 **ALERT type 4** Improvement, methodology, query or suggestion  
0 **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.

