

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx\_a

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\_a

---

Bond precision:    C-C = 0.0089 Å                      Wavelength=0.71075

Cell:                      a=7.6073(3)              b=15.2652(7)              c=20.5263(9)  
                            alpha=90              beta=97.602(1)              gamma=90  
Temperature:              296 K

	Calculated	Reported
Volume	2362.71(18)	2362.71(18)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C10 H30 N2 Na2 O10, 2(C14 H10 Cl2 N O2), 2(H2 O)	C38 H38 Cl4 N4 Na2 O8 , 8(H2O)
Sum formula	C38 H54 Cl4 N4 Na2 O16	C38 H54 Cl4 N4 Na2 O16
Mr	1010.63	1010.63
Dx,g cm-3	1.421	1.421
Z	2	2
Mu (mm-1)	0.340	0.340
F000	1056.0	1056.0
F000'	1057.82	
h,k,lmax	9,19,26	9,19,26
Nref	10769[ 5588]	10695
Tmin,Tmax	0.916,0.960	0.762,0.960
Tmin'	0.915	

Correction method= # Reported T Limits: Tmin=0.762 Tmax=0.960  
AbsCorr = MULTI-SCAN

Data completeness= 1.91/0.99                      Theta(max)= 27.438

R(reflections)= 0.0593( 7586)                      wR2(reflections)= 0.1686( 10695)

S = 1.109                                      Npar= 733

---

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.20	Report
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Na1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Na2	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C14	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C28	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00886	Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	8	Note
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.63A From O13	0.67	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.54A From O13	0.56	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.98A From O10	0.50	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.87A From N1	0.45	eA-3



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	51	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	17	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	10	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT111_ALERT_2_G	ADDSYM Detects New (Pseudo) Centre of Symmetry .	94	%Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem a	94	%Fit
PLAT113_ALERT_2_G	ADDSYM Suggests Possible Pseudo/New Space Group	P21/c	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	17	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	3	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	46%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	26	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	154	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	27	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

- 
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
17 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
15 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  
5 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.

