

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) neu2018

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: neu2018

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Bond precision:    C-C = 0.0013 Å

Wavelength=0.71073

Cell:                a=7.1045(4)                b=8.9553(5)                c=8.9752(6)  
                      alpha=118.307(2)    beta=101.443(2)    gamma=100.500(2)  
Temperature:    293 K

	Calculated	Reported
Volume	466.81(5)	466.80(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C6 H14 N2 O2, 2(H2 O)	?
Sum formula	C6 H18 N2 O4	C6 H18 N2 O4
Mr	182.22	182.22
Dx,g cm-3	1.296	1.296
Z	2	2
Mu (mm-1)	0.107	0.107
F000	200.0	200.0
F000'	200.11	
h,k,lmax	10,13,13	10,13,13
Nref	3390	3374
Tmin,Tmax	0.952,0.962	
Tmin'	0.949	

Correction method= Not given

Data completeness= 0.995

Theta(max)= 32.500

R(reflections)= 0.0352( 3119)

wR2(reflections)= 0.0758( 3374)

S = 1.086

Npar= 162

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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.

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### ● Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O1 --C6 .	6.3 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O2 --C6 .	5.3 s.u.

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### ● Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature . . . . . (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature . . . . . (K)	293 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	2 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	15 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4 Info

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

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

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## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT052_neu2018
;
PROBLEM: Info on Absorption Correction Method    Not Given    Please Do !
RESPONSE: ...
;
_vrf_PLAT230_neu2018
;
PROBLEM: Hirshfeld Test Diff for    O1          --C6          .          6.3 s.u.
RESPONSE: ...
;
# end Validation Reply Form
```

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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.

