

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 2

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

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Bond precision:    C-C = 0.0019 A                      Wavelength=0.71073

Cell:                      a=8.9372(4)              b=8.7877(5)              c=16.8366(8)  
                                    alpha=90              beta=97.888(2)              gamma=90

Temperature:              173 K

|                | Calculated  | Reported    |
|----------------|-------------|-------------|
| Volume         | 1309.79(11) | 1309.79(11) |
| Space group    | P 21/n      | P 21/n      |
| Hall group     | -P 2yn      | -P 2yn      |
| Moiety formula | C14 H18 N6  | C14 H18 N6  |
| Sum formula    | C14 H18 N6  | C14 H18 N6  |
| Mr             | 270.34      | 270.34      |
| Dx,g cm-3      | 1.371       | 1.371       |
| Z              | 4           | 4           |
| Mu (mm-1)      | 0.089       | 0.089       |
| F000           | 576.0       | 576.0       |
| F000'          | 576.15      |             |
| h,k,lmax       | 11,11,21    | 11,10,21    |
| Nref           | 2686        | 2656        |
| Tmin,Tmax      | 0.977,0.982 | 0.920,0.963 |
| Tmin'          | 0.976       |             |

Correction method= # Reported T Limits: Tmin=0.920 Tmax=0.963  
AbsCorr = EMPIRICAL

Data completeness= 0.989                      Theta(max)= 26.415

R(reflections)= 0.0388( 2056)              wR2(reflections)= 0.1032( 2656)

S = 1.058                      Npar= 253

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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**

|                   |   |       |   |      |        |
|-------------------|---|-------|---|------|--------|
| PLAT480_ALERT_4_C | Long H...A H-Bond Reported H2           | ..N4  | . | 2.71 | Ang.   |
| PLAT480_ALERT_4_C | Long H...A H-Bond Reported H4           | ..N5  | . | 2.71 | Ang.   |
| PLAT480_ALERT_4_C | Long H...A H-Bond Reported H11B         | ..N1  | . | 2.78 | Ang.   |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= | 0.600 |   | 6    | Report |

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● **Alert level G**

|                   |  |       |  |     |      |
|-------------------|--|-------|--|-----|------|
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L=        | 0.600 |  | 25  | Note |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity             | ..... |  | 3.6 | Low  |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. |       |  | 9   | 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  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
3 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 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

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## Datablock: 2

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Bond precision: C-C = 0.0033 A                      Wavelength=0.71073

Cell:                      a=9.6759(10)              b=16.3052(8)              c=10.0229(11)  
                            alpha=90                      beta=90                      gamma=90

Temperature:              173 K

|                | Calculated          | Reported            |
|----------------|---------------------|---------------------|
| Volume         | 1581.3(3)           | 1581.3(3)           |
| Space group    | P n m a             | P n m a             |
| Hall group     | -P 2ac 2n           | -P 2ac 2n           |
| Moiety formula | C14 H18 N6, 3(H2 O) | C14 H18 N6, 3(H2 O) |
| Sum formula    | C14 H24 N6 O3       | C14 H24 N6 O3       |
| Mr             | 324.39              | 324.39              |
| Dx,g cm-3      | 1.363               | 1.363               |
| Z              | 4                   | 4                   |
| Mu (mm-1)      | 0.099               | 0.099               |
| F000           | 696.0               | 696.0               |
| F000'          | 696.27              |                     |
| h,k,lmax       | 12,20,12            | 11,19,12            |
| Nref           | 1684                | 1656                |
| Tmin,Tmax      | 0.981,0.987         | 0.912,0.957         |
| Tmin'          | 0.968               |                     |

Correction method= # Reported T Limits: Tmin=0.912 Tmax=0.957

AbsCorr = EMPIRICAL

Data completeness= 0.983

Theta(max)= 26.405

R(reflections)= 0.0493( 857)

wR2(reflections)= 0.1043( 1656)

S = 0.977

Npar= 164

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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

|                   |   |                    |      |    |              |
|-------------------|---|--------------------|------|----|--------------|
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for                   | C3                 | --C9 | .  | 5.8 s.u.     |
| PLAT245_ALERT_2_C | U(iso) H8                                 | Smaller than U(eq) | C8   | by | 0.026 Ang**2 |
| PLAT245_ALERT_2_C | U(iso) H3W                                | Smaller than U(eq) | O2   | by | 0.016 Ang**2 |
| PLAT351_ALERT_3_C | Long C-H (X0.96,N1.08A)                   | C6                 | - H6 | .  | 1.12 Ang.    |
| PLAT480_ALERT_4_C | Long H...A H-Bond Reported                | H1                 | ..01 | .  | 2.62 Ang.    |
| PLAT480_ALERT_4_C | Long H...A H-Bond Reported                | H4A                | ..02 | .  | 2.69 Ang.    |
| PLAT480_ALERT_4_C | Long H...A H-Bond Reported                | H8                 | ..02 | .  | 2.80 Ang.    |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | .....              |      |    | 10.582 Check |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | .....              |      |    | 2.301 Check  |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L=   | 0.600              |      |    | 7 Report     |

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### Alert level G

|                   |  |       |  |  |          |
|-------------------|--|-------|--|--|----------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite |       |  |  | 5 Note   |
| PLAT176_ALERT_4_G | The CIF-Embedded .res File Contains SADI Records |       |  |  | 1 Report |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints               | ..... |  |  | 3 Note   |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L=        | 0.600 |  |  | 10 Note  |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity             | ..... |  |  | 4.0 Low  |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. |       |  |  | 0 Info   |

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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.

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**PLATON version of 18/09/2020; check.def file version of 20/08/2020**



