

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

**Datablock: 281211d\_0m**

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Bond precision:    C-C = 0.0033 Å

Wavelength=0.71073

Cell:                a=7.8700(14)                b=8.0484(15)                c=11.469(2)  
                      alpha=94.770(2)            beta=92.856(3)            gamma=95.972(2)  
Temperature:        291 K

|                        | Calculated    | Reported      |
|------------------------|---------------|---------------|
| Volume                 | 718.8(2)      | 718.8(2)      |
| Space group            | P -1          | P -1          |
| Hall group             | -P 1          | -P 1          |
| Moiety formula         | C16 H12 N4 O4 | C16 H12 N4 O4 |
| Sum formula            | C16 H12 N4 O4 | C16 H12 N4 O4 |
| Mr                     | 324.30        | 324.30        |
| Dx, g cm <sup>-3</sup> | 1.498         | 1.498         |
| Z                      | 2             | 2             |
| Mu (mm <sup>-1</sup> ) | 0.111         | 0.111         |
| F000                   | 336.0         | 336.0         |
| F000'                  | 336.16        |               |
| h,k,lmax               | 9,9,13        | 9,9,13        |
| Nref                   | 2534          | 2499          |
| Tmin,Tmax              | 0.987,0.989   | 0.984,0.989   |
| Tmin'                  | 0.987         |               |

Correction method= MULTI-SCAN

Data completeness= 0.986

Theta(max)= 24.980

R(reflections)= 0.0440( 1199)

wR2(reflections)= 0.1375( 2499)

S = 0.941

Npar= 218

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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

|                   |  |           |
|-------------------|--|-----------|
| PLAT026_ALERT_3_C | Ratio Observed / Unique Reflections too Low .... | 48 Perc.  |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for    C6    --    C7    ..  | 6.56 su   |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for    C8    --    C9    ..  | 5.31 su   |
| PLAT334_ALERT_2_C | Small Average Benzene C-C Dist. C11    -C16      | 1.37 Ang. |

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## Alert level G

PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints .....

2

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0 **ALERT level A** = In general: serious problem  
0 **ALERT level B** = Potentially serious problem  
4 **ALERT level C** = Check and explain  
1 **ALERT level G** = General alerts; check

0 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  
2 ALERT type 3 Indicator that the structure quality may be low  
0 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

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### 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*, 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 31/03/2010; check.def file version of 22/03/2010

