

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hesperetin

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: hesperetin

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Bond precision:    C-C = 0.0030 A

Wavelength=1.54178

Cell:                    a=6.814(3)                    b=8.9657(16)                    c=12.113(3)  
                          alpha=72.322(17)                beta=84.32(2)                    gamma=80.50(2)  
Temperature:            293 K

|                | Calculated       | Reported   |
|----------------|------------------|------------|
| Volume         | 694.5(4)         | 694.4(4)   |
| Space group    | P -1             | P -1       |
| Hall group     | -P 1             | -P 1       |
| Moiety formula | C16 H14 O6, H2 O | ?          |
| Sum formula    | C16 H16 O7       | C16 H16 O7 |
| Mr             | 320.29           | 320.29     |
| Dx,g cm-3      | 1.532            | 1.532      |
| Z              | 2                | 2          |
| Mu (mm-1)      | 1.030            | 1.030      |
| F000           | 336.0            | 336.0      |
| F000'          | 337.23           |            |
| h,k,lmax       | 8,11,14          | 8,11,14    |
| Nref           | 2760             | 2694       |
| Tmin,Tmax      |                  |            |
| Tmin'          |                  |            |

Correction method= Not given

Data completeness= 0.976

Theta(max)= 72.635

R(reflections)= 0.0506( 2455)

wR2(reflections)= 0.1360( 2694)

S = 1.062

Npar= 223

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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 A

EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing  
Crystal habit description.  
The following tests will not be performed.  
CRYSR\_01

DIFF003\_ALERT\_1\_A \_diffrn\_measurement\_device\_type is missing

Diffractometer make and type. Replaces \_diffrn\_measurement\_type.

PLAT183\_ALERT\_1\_A Missing \_cell\_measurement\_reflms\_used Value .... Please Do !  
PLAT184\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_min Value ..... Please Do !  
PLAT185\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_max Value ..... Please Do !

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### 🟡 Alert level B

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 0.98 eA-3

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### 🟢 Alert level C

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
The relevant atom site should be identified.

PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given Please Do !  
PLAT053\_ALERT\_1\_C Minimum Crystal Dimension Missing (or Error) ... Please Check  
PLAT054\_ALERT\_1\_C Medium Crystal Dimension Missing (or Error) ... Please Check  
PLAT055\_ALERT\_1\_C Maximum Crystal Dimension Missing (or Error) ... Please Check  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 3.44 Report  
PLAT250\_ALERT\_2\_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.428 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 40 Report  
PLAT913\_ALERT\_3\_C Missing # of Very Strong Reflections in FCF .... 4 Note

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### 🟣 Alert level G

PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check  
PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 1 Note  
PLAT793\_ALERT\_4\_G Model has Chirality at C6 (Centro SPGR) R Verify  
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 26 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 8 Info

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

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

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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 03/05/2019; check.def file version of 29/04/2019**

