checkCIF/PLATON report

Structure factors have been supplied for datablock(s) aldosteron

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: aldosteron

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Bond precision:  C-C = 0.0020 A          Wavelength=1.54184

Cell:           a=12.1724(5)    b=5.9607(2)         c=13.1250(5)
                alpha=90        beta=107.547(5)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          907.99(6)                 907.98(6)
Space group     P 21                      P 21
Hall group      P 2yb                     P 2yb
Moiety formula  C21 H28 O5, H2 O          C21 H28 O5, H2 O
Sum formula     C21 H30 O6                C21 H30 O6
Mr              378.45                    378.45
Dx,g cm-3       1.384                     1.384
Z               2                         2
Mu (mm-1)       0.822                     0.822
F000            408.0                     408.0
F000'           409.31
h,k,lmax        15,7,16                   15,7,16
Nref            3728[ 2051]               3705
Tmin,Tmax       0.862,0.936               0.889,1.000
Tmin'           0.781

Correction method= # Reported T Limits: Tmin=0.889 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.81/0.99      Theta(max)= 74.700

R(reflections)= 0.0327( 3559)     wR2(reflections)= 0.0863( 3705)

S = 1.042                 Npar= 257
```

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 B

PLAT035_ALERT_1_B _chemical_absolute_configuration info Not given Please Do !

Alert level C

PLAT414_ALERT_2_C Short Intra D-H..H-X H4 .. H17B .. 1.94 Ang.

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT398_ALERT_2_G Deviating C-O-C Angle from 120 Deg for O2 107.1 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle from 120 Deg for O3 106.1 Degree
PLAT791_ALERT_4_G The Model has Chirality at C4 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G The Model has Chirality at C10 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G The Model has Chirality at C11 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G The Model has Chirality at C12 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G The Model has Chirality at C14 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G The Model has Chirality at C15 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G The Model has Chirality at C18 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G The Model has Chirality at C19 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G The Model has Chirality at C21 (Chiral SPGR) R Verify
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 5 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 19 Note

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

1 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
0 ALERT type 3 Indicator that the structure quality may be low
11 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock aldosteron - ellipsoid plot