

# 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

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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 B**

PLAT035\_ALERT\_1\_B \_chemical\_absolute\_configuration info Not given Please Do !

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**Alert level C**

PLAT414\_ALERT\_2\_C Short Intra D-H..H-X H4 .. H17B .. 1.94 Ang.

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**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

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

