

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: Compound\_I

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Bond precision:    C-C = 0.0087 A                      Wavelength=0.71073

Cell:                      a=6.691(2)              b=19.642(4)              c=7.719(3)  
                                    alpha=90              beta=92.123(2)              gamma=90

Temperature:              298 K

	Calculated	Reported
Volume	1013.8(5)	1013.8(5)
Space group	P 21	P21
Hall group	P 2yb	P2yb
Moiety formula	C26 H20 N2 O2	C26 H20 N2 O2
Sum formula	C26 H20 N2 O2	C26 H20 N2 O2
Mr	392.44	392.44
Dx,g cm-3	1.286	1.286
Z	2	2
Mu (mm-1)	0.082	0.082
F000	412.0	412.0
F000'	412.17	
h,k,lmax	8,26,10	8,26,10
Nref	5099[ 2621]	3803
Tmin,Tmax	0.979,0.984	0.984,0.991
Tmin'	0.978	

Correction method= EMPIRICAL

Data completeness= 1.45/0.75                      Theta(max)= 28.400

R(reflections)= 0.0936( 2439)                      wR2(reflections)= 0.2105( 3803)

S = 1.056                                      Npar= 271

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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**

PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0087 Ang.

● **Alert level G**

PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF Please Do !  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 1 Report  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large. 0.15 Report  
PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
4 **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  
1 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

## Datablock: Compound\_II

Bond precision: C-C = 0.0038 A Wavelength=0.71073  
Cell: a=14.121(5) b=10.361(4) c=14.130(5)  
alpha=90 beta=117.632(7) gamma=90  
Temperature: 298 K

	Calculated	Reported
Volume	1831.5(12)	1831.5(12)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P2yn
Moiety formula	C22 H20 N2 O2	C22 H20 N2 O2
Sum formula	C22 H20 N2 O2	C22 H20 N2 O2
Mr	344.40	344.40
Dx,g cm-3	1.249	1.249
Z	4	4
Mu (mm-1)	0.081	0.081
F000	728.0	728.0
F000'	728.30	
h,k,lmax	18,13,18	18,13,18
Nref	4581	4499
Tmin,Tmax	0.981,0.985	0.981,0.985
Tmin'	0.981	

Correction method= EMPIRICAL

Data completeness= 0.982

Theta(max)= 28.340

R(reflections)= 0.0626( 1969)

wR2(reflections)= 0.2079( 4499)

S = 0.954

Npar= 235

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**test-name\_ALERT\_alert-type\_alert-level.**

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#### Alert level C

PLAT026\_ALERT\_3\_C Ratio Observed / Unique Reflections too Low ....

44 %



#### Alert level G

PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF

Please Do !

PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical

? Check

PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL

2014 Note

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## Datablock: Compound\_III

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Bond precision: C-C = 0.0046 A

Wavelength=0.71073

Cell: a=7.0564(17)

b=7.4268(17)

c=18.270(4)

alpha=90.823(5)

beta=91.860(5)

gamma=109.877(3)

Temperature: 298 K

	Calculated	Reported
Volume	899.6(4)	899.6(4)
Space group	P -1	P-1
Hall group	-P 1	-P1
Moiety formula	2(C21 H20 N2 O2), C2 H8 O	C44 H48 N4 O5
Sum formula	C44 H48 N4 O5	C44 H48 N4 O5
Mr	712.86	712.86
Dx,g cm-3	1.316	1.316
Z	1	1
Mu (mm-1)	0.086	0.086
F000	380.0	380.0
F000'	380.16	
h,k,lmax	8,8,22	8,8,22
Nref	3346	3277
Tmin,Tmax	0.981,0.985	0.981,0.985
Tmin'	0.981	

Correction method= EMPIRICAL

Data completeness= 0.979                      Theta(max)= 25.500


R(reflections)= 0.0769( 2220)              wR2(reflections)= 0.2519( 3277)

S = 1.022                                      Npar= 249


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**test-name\_ALERT\_alert-type\_alert-level**.  
Click on the hyperlinks for more details of the test.

 **Alert level A**

PLAT414\_ALERT\_2\_A Short Intra D-H..H-X              H3S    .. H22A    ..              1.58 Ang.


 **Alert level B**

PLAT420\_ALERT\_2\_B D-H Without Acceptor              O3    -    H3S    ...              Please Check

 **Alert level C**

RFACR01\_ALERT\_3\_C The value of the weighted R factor is > 0.25  
Weighted R factor given 0.252

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	Low	.....	0.979	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	.....	.....	0.0046	Ang.
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H9	.. H22B ..	2.10	Ang.
PLAT414_ALERT_2_C	Short Intra D-H..H-X	H3S	.. H22C ..	1.91	Ang.

 **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF		Please Do !
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.15	Report

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C20 .. C22 .. 3.20 Ang.  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 1 Note  
PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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## Datablock: Compound\_IV

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Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=4.9084(17) b=14.926(5) c=12.013(4)  
alpha=90 beta=99.761(7) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	867.4(5)	867.4(5)
Space group	P n	Pn
Hall group	P -2yac	?
Moiety formula	C21 H18 N2 O3	C21 H18 N2 O3
Sum formula	C21 H18 N2 O3	C21 H18 N2 O3
Mr	346.37	346.37
Dx,g cm-3	1.326	1.330
Z	2	2
Mu (mm-1)	0.090	0.090
F000	364.0	364.0
F000'	364.17	
h,k,lmax	6,18,14	6,18,14
Nref	3398[ 1708]	2880
Tmin,Tmax	0.986,0.988	0.986,0.988
Tmin'	0.986	

Correction method= EMPIRICAL

Data completeness= 1.69/0.85 Theta(max)= 25.990

R(reflections)= 0.0536( 2428) wR2(reflections)= 0.1565( 2880)

S = 1.028 Npar= 235

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● **Alert level C**

PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18) .....	7.27	Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.36	Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for N2 -- C10 ..	5.5	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C17 -- C18 ..	6.5	su
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.0043	Ang.

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● **Alert level G**

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF		Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.12	Report
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C12	Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL		2014 Note

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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*, 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 20/08/2014; check.def file version of 18/08/2014**

