

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) p12063

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: p12063

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Bond precision:    C-C = 0.0044 Å                      Wavelength=1.54178

Cell:                      a=14.4057(4)              b=14.9409(3)              c=22.8735(7)  
                            alpha=90                      beta=90                      gamma=90  
Temperature:              100 K

	Calculated	Reported
Volume	4923.2(2)	4923.2(2)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C45 H62 N4 O15, C H Cl3	C45 H62 N4 O15, C H Cl3
Sum formula	C46 H63 Cl3 N4 O15	C46 H63 Cl3 N4 O15
Mr	1018.35	1018.35
Dx,g cm-3	1.374	1.374
Z	4	4
Mu (mm-1)	2.287	2.287
F000	2152.0	2152.0
F000'	2162.91	
h,k,lmax	18,18,28	17,18,28
Nref	10062[ 5556]	10050
Tmin,Tmax	0.606,0.852	0.748,1.000
Tmin'	0.538	

Correction method= # Reported T Limits: Tmin=0.748 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.81/1.00                      Theta(max)= 74.480

R(reflections)= 0.0422( 9228)                      wR2(reflections)= 0.1135( 10050)

S = 1.030                      Npar= 650

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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**

PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C46	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00438	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H1B ..N2 .	2.68	Ang.

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**Alert level G**

PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C5 -C10 .	1.43	Ang.
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3	108.5	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact O14 ..C46	2.97	Ang.
	x,y,z =	1_555	Check
PLAT791_ALERT_4_G	Model has Chirality at C12 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C18 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C21 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C22 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C23 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C24 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C25 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C26 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C27 (Sohnke SpGr)	S	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	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	6	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.8	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
18 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 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  
12 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.

