## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 22dub\_vj04

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: 22dub\_vj04

Bond precision:	C-C = 0.0022 A	Wavelength=1.54184			
Cell:	a=6.7326(2) alpha=90		c=25.2164(6) gamma=90		
Temperature:	153 K		-		
	Calculated	Reported			
Volume	1366.74(6)	1366.74(6	)		
Space group	P 21/n	P 1 21/n	1		
Hall group	-P 2yn	-P 2yn			
Moiety formula	C18 H13 N O S	C18 H13 N	O S		
Sum formula	C18 H13 N O S	C18 H13 N	O S		
Mr	291.35	291.35			
Dx,g cm-3	1.416	1.416			
Z	4	4			
Mu (mm-1)	2.070	2.070			
F000	608.0	608.0			
F000′	610.88				
h,k,lmax	8,9,31	7,9,31			
Nref	2659	2494			
Tmin,Tmax	0.685,0.747	0.831,1.0	00		
Tmin'	0.622				
Correction method= # Reported T Limits: Tmin=0.831 Tmax=1.000 AbsCorr = GAUSSIAN					
Data completenes	ss= 0.938	Theta(max) = 71.544	4		
R(reflections)= 0.0355( 2342)			wR2(reflections)= 0.0970(2494)		
S = 1.062	Npar= 1	191			

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 C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .	0.971 Why?
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	62 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers	1 Check

## Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	70 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF	2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	1.6 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	12 Info

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
5 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
5 ALERT type 3 Indicator that the structure quality may be low
1 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 19/02/2022; check.def file version of 19/02/2022

Datablock 22dub\_vj04 - ellipsoid plot

