

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 210118wyh_1_0m

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: 210118wyh_1_0m

Bond precision:	C-C = 0.0044 Å	Wavelength=1.34139	
Cell:	a=9.47499(10)	b=9.47499(10)	c=70.0389(7)
	alpha=90	beta=90	gamma=120
Temperature:	193 K		
	Calculated	Reported	
Volume	5445.37(13)	5445.37(13)	
Space group	P 61	P 61	
Hall group	P 61	P 61	
Moiety formula	C21 H19 N O3	C21 H19 N O3	
Sum formula	C21 H19 N O3	C21 H19 N O3	
Mr	333.37	333.37	
Dx, g cm-3	1.220	1.220	
Z	12	12	
Mu (mm-1)	0.419	0.423	
F000	2112.0	2112.0	
F000'	2116.84		
h, k, lmax	11, 11, 85	11, 11, 85	
Nref	6915[3488]	6910	
Tmin, Tmax	0.975, 0.987	0.691, 0.751	
Tmin'	0.967		

Correction method= # Reported T Limits: Tmin=0.691 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 1.98/1.00 Theta(max)= 54.891

R(reflections)= 0.0332(6259) wR2(reflections)= 0.0840(6910)

S = 1.031 Npar= 455

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

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00442 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H18A ..H21D . 2.13 Ang.
x, -1+y, z = 1_545 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C21 H19 N O3

● Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00070 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C12 ..C12A 3.11 Ang.
-1+x,y,z = 1_455 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C21 H19 N O3
PLAT791_ALERT_4_G Model has Chirality at C1 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C1A (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C2 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C2A (Sohnke SpGr) R Verify
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT984_ALERT_1_G The C-f' = 0.0148 Deviates from the B&C-Value 0.0137 Check
PLAT984_ALERT_1_G The N-f' = 0.0253 Deviates from the B&C-Value 0.0241 Check
PLAT984_ALERT_1_G The O-f' = 0.0412 Deviates from the B&C-Value 0.0389 Check

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
13 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
7 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

