

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: p21c_71

Bond precision:	C-C = 0.0020 A	Wavelength=0.71073
Cell:	a=7.5504(1) b=19.8885(3) c=11.6408(2)	
	alpha=90 beta=105.4479(6) gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	1684.90(4)	1684.90(4)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C34 H30 F8 K2 N4 O2	0.5(C34 H30 F8 K2 N4 O2)
Sum formula	C34 H30 F8 K2 N4 O2	C17 H15 F4 K N2 O
Mr	756.82	378.41
Dx,g cm-3	1.492	1.492
Z	2	4
Mu (mm-1)	0.364	0.364
F000	776.0	776.0
F000'	777.28	
h,k,lmax	10,28,16	10,28,16
Nref	10127[5197]	8299
Tmin,Tmax	0.957,0.964	0.690,0.746
Tmin'	0.930	

Correction method= # Reported T Limits: Tmin=0.690 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.60/0.82 Theta(max)= 30.330

R(reflections)= 0.0262(7977) wR2(reflections)= 0.0653(8299)

S = 1.029 Npar= 475

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: `_refine_ls_abs_structure_Flack` 0.691
From the CIF: `_refine_ls_abs_structure_Flack_su` 0.017
PLAT907_ALERT_2_C Flack $x > 0.5$, Structure needs to be Inverted? . 0.69 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT033_ALERT_4_G Flack x Value Deviates $> 3.0 * \sigma$ from Zero . 0.691 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 6 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.27 Ratio

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

2 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
0 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
2 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 24/11/2016; check.def file version of 23/11/2016

Datablock p21c_71 - ellipsoid plot

