

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rpcjmg

No syntax errors found. CIF dictionary Interpreting this report

Datablock: rpcjmg

Bond precision: C-C = 0.0021 Å Wavelength=1.54184

Cell: a=9.5898(11) b=15.6530(15) c=11.0541(13)
 alpha=90 beta=115.637(14) gamma=90

Temperature: 90 K

	Calculated	Reported
Volume	1496.0(3)	1496.0(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C14 H14 F3 N O5	C14 H14 F3 N O5
Sum formula	C14 H14 F3 N O5	C14 H14 F3 N O5
Mr	333.26	333.26
Dx, g cm ⁻³	1.480	1.480
Z	4	4
Mu (mm ⁻¹)	1.191	1.191
F000	688.0	688.0
F000'	690.91	
h,k,lmax	11,19,13	11,19,13
Nref	3044	2959
Tmin,Tmax	0.744,0.842	0.830,1.558
Tmin'	0.515	

Correction method= GAUSSIAN

Data completeness= 0.972 Theta(max)= 74.490

R(reflections)= 0.0355(2600) wR2(reflections)= 0.0930(2959)

S = 1.044 Npar= 211

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

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=	0.600	9
PLAT912_ALERT_4_C Missing # of FCF Reflections Above STh/L=	0.600	76
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF		1



Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT128_ALERT_4_G	Alternate Setting of Space-group P21/c	P21/n
PLAT793_ALERT_4_G	The Model has Chirality at C4 (Verify)	S
PLAT793_ALERT_4_G	The Model has Chirality at C5 (Verify)	R

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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
4 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
4 ALERT type 4 Improvement, methodology, query or suggestion
1 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*, 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.

