

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: rpcjmf

Bond precision:	C-C = 0.0067 A	Wavelength=1.54184	
Cell:	a=4.499(2)	b=11.188(6)	c=13.464(12)
	alpha=91.14(8)	beta=97.51(7)	gamma=90.08(4)
Temperature:	90 K		
	Calculated	Reported	
Volume	671.8(8)	671.7(8)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C14 H12 F3 N O4	C14 H12 F3 N O4	
Sum formula	C14 H12 F3 N O4	C14 H12 F3 N O4	
Mr	315.25	315.25	
Dx,g cm-3	1.559	1.559	
Z	2	2	
Mu (mm-1)	1.235	1.235	
F000	324.0	324.0	
F000'	325.36		
h,k,lmax	5,13,15	5,13,16	
Nref	2383	3356	
Tmin,Tmax	0.877,0.911	0.950,1.537	
Tmin'	0.391		

Correction method= GAUSSIAN

Data completeness= 1.408 Theta(max)= 66.600

R(reflections)= 0.1029(2833) wR2(reflections)= 0.3727(3356)

S = 1.757 Npar= 202

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 B

RFACR01_ALERT_3_B The value of the weighted R factor is > 0.35

Weighted R factor given 0.373

PLAT021_ALERT_1_B Ratio Unique / Expected Reflections too High ... 1.408

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full Low 0.946

PLAT084_ALERT_2_B High wR2 Value	0.37
PLAT149_ALERT_3_B su on the alpha Angle is Too Large	0.08 Deg.
PLAT149_ALERT_3_B su on the beta Angle is Too Large	0.07 Deg.

● Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
 _refine_diff_density_min given = -0.713
 Test value = -0.675

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
 The relevant atom site should be identified.

RFACG01_ALERT_3_C The value of the R factor is > 0.10
 R factor given 0.103

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density	-0.71 eA-3
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.0067 Ang
PLAT431_ALERT_2_C Short Inter HL..A Contact F21 .. O1 ..	2.85 Ang.

● Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF	?
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size	0.76 mm
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large.	0.20

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 6 **ALERT level B** = A potentially serious problem, consider carefully
 - 6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 3 **ALERT level G** = General information/check it is not something unexpected
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- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 6 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
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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.

