

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rpcjmd

No syntax errors found. CIF dictionary Interpreting this report

Datablock: rpcjmd

Bond precision: C-C = 0.0082 Å Wavelength=1.54184

Cell: a=7.8560(14) b=8.957(2) c=10.209(3)
 alpha=91.807(19) beta=98.090(18) gamma=101.202(17)

Temperature: 90 K

	Calculated	Reported
Volume	696.4(3)	696.4(3)
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	1.503	1.503
Z	2	2
Mu (mm-1)	1.192	1.192
F000	324.0	324.0
F000'	325.36	
h,k,lmax	9,10,12	9,10,12
Nref	2465	2415
Tmin,Tmax	0.734,0.942	0.414,1.000
Tmin'	0.577	

Correction method= MULTI-SCAN

Data completeness= 0.980 Theta(max)= 66.590

R(reflections)= 0.1165(1821) wR2(reflections)= 0.3692(2415)

S = 1.491 Npar= 201

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 0.369

PLAT084_ALERT_2_B High wR2 Value 0.37

● **Alert level C**

DIFMX01_ALERT_2_C The maximum difference density is > 0.1*ZMAX*0.75
 _refine_diff_density_max given = 0.693
 Test value = 0.675
DIFMX02_ALERT_1_C The maximum 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 0.116
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.979
PLAT082_ALERT_2_C High R1 Value 0.12
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.69 eA-3
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0082 Ang
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.595 51

● **Alert level G**

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ?
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.20
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 61 Perc.

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
9 **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
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
0 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.

