

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_ydg\_lcf\_zq\_1\_0m\_a

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: mo\_ydg\_lcf\_zq\_1\_0m\_a

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Bond precision:      C-C = 0.0033 A      Wavelength=0.71073

Cell:                      a=4.8999 (1)              b=10.4794 (3)              c=31.2171 (9)  
                                    alpha=90              beta=90              gamma=90

Temperature:              302 K

	Calculated	Reported
Volume	1602.94 (7)	1602.94 (7)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C12 H17 F N6 O4 S, H2 O	C12 H17 F N6 O4 S, H2 O
Sum formula	C12 H19 F N6 O5 S	C12 H19 F N6 O5 S
Mr	378.39	378.39
Dx, g cm <sup>-3</sup>	1.568	1.568
Z	4	4
Mu (mm <sup>-1</sup> )	0.253	0.253
F000	792.0	792.0
F000'	792.90	
h, k, lmax	6, 13, 40	6, 13, 40
Nref	3689 [ 2183]	3687
Tmin, Tmax	0.927, 0.973	0.645, 0.746
Tmin'	0.895	

Correction method= # Reported T Limits: Tmin=0.645 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.69/1.00              Theta (max)= 27.489

R(reflections)= 0.0341 ( 3070)

wR2(reflections)=  
0.0806 ( 3687)

S = 1.031

Npar= 240

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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.

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	7	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	3	Note
PLAT791_ALERT_4_G	Model has Chirality at C4 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C5 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C13 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C14 (Sohnke SpGr)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	4	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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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
- 0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 12 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  - 2 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
  - 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* 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.

