

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 13631sadabs\_large\_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: 13631sadabs\_large\_a

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Bond precision:      C-C = 0.0060 Å

Wavelength=0.71073

Cell:                      a=11.4394(5)                      b=11.4703(5)                      c=17.3113(7)  
                              alpha=87.411(2)                      beta=81.367(2)                      gamma=84.321(2)  
Temperature:              200 K

|                        | Calculated         | Reported           |
|------------------------|--------------------|--------------------|
| Volume                 | 2233.65(17)        | 2233.65(17)        |
| Space group            | P -1               | P -1               |
| Hall group             | -P 1               | -P 1               |
| Moiety formula         | C14 H12 F3 N3 O3 S | C14 H12 F3 N3 O3 S |
| Sum formula            | C14 H12 F3 N3 O3 S | C14 H12 F3 N3 O3 S |
| Mr                     | 359.33             | 359.33             |
| Dx, g cm <sup>-3</sup> | 1.603              | 1.603              |
| Z                      | 6                  | 6                  |
| Mu (mm <sup>-1</sup> ) | 0.272              | 0.272              |
| F000                   | 1104.0             | 1104.0             |
| F000'                  | 1105.44            |                    |
| h,k,lmax               | 15,15,23           | 15,15,23           |
| Nref                   | 11205              | 11144              |
| Tmin,Tmax              | 0.985,0.993        | 0.986,0.995        |
| Tmin'                  | 0.977              |                    |

Correction method= # Reported T Limits: Tmin=0.986 Tmax=0.995  
AbsCorr = GAUSSIAN

Data completeness= 0.995

Theta(max)= 28.375

R(reflections)= 0.0759( 5925)

wR2(reflections)=  
0.2298( 11144)

S = 1.011

Npar= 756

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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 B

PLAT220\_ALERT\_2\_B NonSolvent Resd 4 C Ueq(max)/Ueq(min) Range 7.4 Ratio

**Author Response: This is due to disorder.**

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### Alert level C

PLAT213\_ALERT\_2\_C Atom F3\_3 has ADP max/min Ratio ..... 3.4 prolat  
PLAT213\_ALERT\_2\_C Atom F3'\_3 has ADP max/min Ratio ..... 3.4 prolat  
PLAT222\_ALERT\_3\_C NonSolvent Resd 4 H Uiso(max)/Uiso(min) Range 4.9 Ratio  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of N1\_1 Check  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00604 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 7.166 Check

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### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 56 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or U(i,j) Restrained non-H Atoms 24 Report  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 3 Report  
PLAT174\_ALERT\_4\_G The CIF-Embedded .res File Contains FLAT Records 1 Report  
PLAT175\_ALERT\_4\_G The CIF-Embedded .res File Contains SAME Records 1 Report  
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 3 Report  
PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 1 Report  
PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 1 Report  
PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for F2'\_3 --C9\_3 . 5.3 s.u.  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C9\_3 Check  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C9\_1 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1) 13% Note  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 4) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 3) 29.95 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 4) 6.05 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O2\_2 ..C5\_1 . 3.01 Ang.  
x,y,z = 1\_555 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O2\_3 ..C11'\_2 . 2.78 Ang.  
1-x,1-y,1-z = 2\_666 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O2\_3 ..C12'\_2 . 2.90 Ang.  
1-x,1-y,1-z = 2\_666 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O2'\_2 ..C5\_3 . 2.94 Ang.  
x,y,z = 1\_555 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O3'\_2 ..C12\_1 . 2.86 Ang.  
-x,1-y,-z = 2\_565 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C10\_3 ..C4'\_2 . 3.04 Ang.  
x,y,z = 1\_555 Check  
PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 446 Note

|                   |                                                  |                      |        |       |
|-------------------|--------------------------------------------------|----------------------|--------|-------|
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L=        | 0.600                | 60     | Note  |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File |                      | 1      | Note  |
|                   | 2 5 1,                                           |                      |        |       |
| PLAT965_ALERT_2_G | The SHELXL WEIGHT Optimisation has not Converged |                      | Please | Check |
| PLAT969_ALERT_5_G | The 'Henn et al.' R-Factor-gap value .....       | 4.872                | Note   |       |
|                   | Predicted wR2: Based on SigI**2                  | 4.72 or SHELX Weight | 22.73  |       |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. |                      | 1      | Info  |
| PLAT992_ALERT_5_G | Repd & Actual _reflns_number_gt Values Differ by |                      | 3      | Check |

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
18 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  
10 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

Datablock 13631sadabs\_large\_a - ellipsoid plot

