checkCIF/PLATON report

Structure factors have been supplied for datablock(s) litfsa_eips_1_1.5

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: litfsa_eips_1_1.5

```
Bond precision:    C-C = 0.0050 A              Wavelength=0.71073

Cell:             a=18.9850(9)     b=8.7718(4)           c=21.8241(12)
                  alpha=90         beta=111.777(6)       gamma=90
Temperature:      223 K

                  Calculated                   Reported
Volume            3375.1(3)                    3375.1(3)
Space group       P 21/c                       P 1 21/c 1
Hall group        -P 2ybc                      -P 2ybc
Moiety formula    C14 H24 F12 Li2 N2 O12 S6    C14 H24 F12 Li2 N2 O12 S6
Sum formula       C14 H24 F12 Li2 N2 O12 S6    C14 H24 F12 Li2 N2 O12 S6
Mr                846.59                       846.59
Dx,g cm-3         1.666                        1.666
Z                 4                            4
Mu (mm-1)         0.524                        0.524
F000              1712.0                       1712.0
F000'             1716.39
h,k,lmax          26,12,30                     26,12,30
Nref              9917                         9251
Tmin,Tmax                                      0.963,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=0.963 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.933              Theta(max)= 30.062

                                                   wR2(reflections)=
R(reflections)= 0.0467( 6673)                      0.1534( 9251)

S = 0.932                     Npar= 484
```

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

```
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...      Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...      Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...      Please Check
PLAT213_ALERT_2_C Atom F1            has ADP max/min Ratio .....      3.4 prolat
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      O00E Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      O00H Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      S02 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      S04 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      S05 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      S06 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Li01 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............      0.005 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.186 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).      10 Note
```

⚪ Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         2 Info
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F2       --C4       .     11.9 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F4       --C4       .     12.4 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F5       --C4       .     13.1 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C00X Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C4 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C00Y Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C015 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O00L       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O00P       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O00V       Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )      10% Note
PLAT431_ALERT_2_G Short Inter HL..A Contact  F00O    ..O1       .      2.81 Ang.
                                            x,1+y,z  =      1_565 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F1      ..F1       .      2.62 Ang.
                                            2-x,-y,1-z =      3_756 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      67 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      655 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       0 Info
```

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

```
 3 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
 4 ALERT type 3 Indicator that the structure quality may be low
12 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check
```

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.

PLATON version of 18/05/2022; check.def file version of 17/05/2022