

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) litfsa_msl

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_msl

Bond precision:	C-C = 0.0090 A	Wavelength=0.71073
Cell:	a=17.8545(10)	b=12.6864(7) c=14.6399(8)
	alpha=90	beta=90 gamma=90
Temperature:	223 K	
	Calculated	Reported
Volume	3316.1(3)	3316.1(3)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C14 H20 F12 Li2 N2 O12 S6	C13.999 H19.995 F12 Li2 N2 O12 S6
Sum formula	C14 H20 F12 Li2 N2 O12 S6	C14 H20 F12 Li2 N2 O12 S6
Mr	842.55	842.56
Dx, g cm-3	1.688	1.688
Z	4	4
Mu (mm-1)	0.533	0.533
F000	1696.0	1696.0
F000'	1700.35	
h,k,lmax	25,17,20	24,17,20
Nref	9856[5104]	8471
Tmin,Tmax		0.890,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.890 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.66/0.86 Theta(max)= 30.193

R(reflections)= 0.0455(7027)	wR2(reflections)= 0.1310(8471)
S = 1.030	Npar= 453

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
 From the CIF: `_refine_ls_abs_structure_Flack` 0.410
 From the CIF: `_refine_ls_abs_structure_Flack_su` 0.020

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
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
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	07 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	018 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	034 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	035 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	045 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C4 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C8 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C41 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S1 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S11 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S13 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S26 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S28 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S43 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Li47 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.009 Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	7 Note

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C10 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C14 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C25 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C29 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3 Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C40 Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1 Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6 Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2BC Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2BD Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3 Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4BC Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4BD Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8BD Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8BE Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8BF Constrained at	0.666 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39A Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39B Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40 Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41A Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41B Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46A Constrained at	0.75 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H46B	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46C	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2AA	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2AB	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4AA	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4AB	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8AA	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8AB	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8AC	Constrained at	0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46E	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46F	Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		4%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		14	Note
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4			Please Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C46 --C6		1.79	Ang.
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		341	Note
PLAT915_ALERT_3_G	No Flack x Check Done: Low Friedel Pair Coverage		78	%
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
 22 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 48 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 21 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
 40 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.

