

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ip276

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: ip276

Bond precision: C-C = 0.0025 A Wavelength=0.71073

Cell: a=9.6687(19) b=9.948(2) c=19.611(4)
 alpha=93.77(3) beta=91.33(3) gamma=90.96(3)

Temperature: 153 K

	Calculated	Reported
Volume	1881.4(7)	1881.3(6)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C38 H54 Li2 N4 O2	?
Sum formula	C38 H54 Li2 N4 O2	C38 H54 Li2 N4 O2
Mr	612.73	612.73
Dx,g cm-3	1.082	1.082
Z	2	2
Mu (mm-1)	0.066	0.066
F000	664.0	664.0
F000'	664.23	
h,k,lmax	12,12,24	12,12,24
Nref	7689	7395
Tmin,Tmax	0.961,0.974	
Tmin'	0.961	

Correction method= Not given

Data completeness= 0.962 Theta(max)= 26.370

R(reflections)= 0.0520(5226) wR2(reflections)= 0.1347(7395)

S = 1.013 Npar= 469

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

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	Low	0.962	Note
PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min) Range	4.2	Ratio
PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C36	-- C37 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C37	-- C38 ..	0.19	Ang.
PLAT242_ALERT_2_C	Low	Ueq	as Compared to Neighbors for	C13	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		9.004	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		2.152	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600		221	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		3	Note

● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF		Please	Do !
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal		0.03000	Degree
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	11	Note
PLAT371_ALERT_2_G	Long	C(sp2)-C(sp1) Bond	C23 - C24 ...	1.43	Ang.
PLAT371_ALERT_2_G	Long	C(sp2)-C(sp1) Bond	C3 - C4 ...	1.44	Ang.
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	59	Do !
	N1	-C1 -C2 -C3	165.00 11.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	60	Do !
	N2	-C1 -C2 -C3	-15.00 12.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	61	Do !
	LI1	-C1 -C2 -C3	92.00 12.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	62	Do !
	C1	-C2 -C3 -C4	-72.00 15.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	63	Do !
	C2	-C3 -C4 -C9	-41.00 7.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	64	Do !
	C2	-C3 -C4 -C5	138.00 7.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	146	Do !
	N4	-C21 -C22 -C23	-71.00 3.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	147	Do !
	N3	-C21 -C22 -C23	107.00 3.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	148	Do !
	LI2	-C21 -C22 -C23	-142.00 2.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	149	Do !
	C21	-C22 -C23 -C24	-7.00 7.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	150	Do !
	C22	-C23 -C24 -C25	22.00 5.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete	1-2-3 or 2-3-4	Linear Torsion Angle ... #	151	Do !
	C22	-C23 -C24 -C29	-158.00 5.00 1.555 1.555 1.555	1.555	
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C38'	-- C39'	.	1.75	Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#		2	Note
	C38	H54 Li2 N4 O2			
PLAT793_ALERT_4_G	The Model has Chirality at C1	(Centro SPGR)		S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at C21	(Centro SPGR)		S	Verify
PLAT899_ALERT_4_G	SHELXL97	is Deprecated and Succeeded by SHELXL		2014	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Th(Min)	...		1	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		71	Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
10 **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

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
7 ALERT type 3 Indicator that the structure quality may be low
19 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*, 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 21/06/2015; check.def file version of 21/06/2015

